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NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	JAN 17	Pre-1988 INPI data added to MARPAT
NEWS 4	FEB 21	STN AnaVist, Version 1.1, lets you share your STN AnaVist visualization results
NEWS 5	FEB 22	The IPC thesaurus added to additional patent databases on STN
NEWS 6	FEB 22	Updates in EPFULL; IPC 8 enhancements added
NEWS 7	FEB 27	New STN AnaVist pricing effective March 1, 2006
NEWS 8	MAR 03	Updates in PATDPA; addition of IPC 8 data without attributes
NEWS 9	MAR 22	EMBASE is now updated on a daily basis
NEWS 10	APR 03	New IPC 8 fields and IPC thesaurus added to PATDPAFULL
NEWS 11	APR 03	Bibliographic data updates resume; new IPC 8 fields and IPC thesaurus added in PCTFULL
NEWS 12	APR 04	STN AnaVist $500 visualization usage credit offered
NEWS 13	APR 12	LINSPEC, learning database for INSPEC, reloaded and enhanced
NEWS 14	APR 12	Improved structure highlighting in FQHIT and QHIT display in MARPAT
NEWS 15	APR 12	Derwent World Patents Index to be reloaded and enhanced during second quarter; strategies may be affected
NEWS 16	MAY 10	CA/CAplus enhanced with 1900-1906 U.S. patent records
NEWS 17	MAY 11	KOREAPAT updates resume
NEWS 18	MAY 19	Derwent World Patents Index to be reloaded and enhanced
NEWS 19	MAY 30	IPC 8 Rolled-up Core codes added to CA/CAplus and USPATFULL/USPAT2
NEWS 20	MAY 30	The F-Term thesaurus is now available in CA/CAplus
NEWS 21	JUN 02	The first reclassification of IPC codes now complete in INPADOC
NEWS EXPRESS		FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005. V8.0 AND V8.01 USERS CAN OBTAIN THE UPGRADE TO V8.01a AT http://download.cas.org/express/v8.0-Discover/
NEWS HOURS		STN Operating Hours Plus Help Desk Availability
NEWS LOGIN		Welcome Banner and News Items
NEWS IPC8		For general information regarding STN implementation of IPC 8
NEWS X25		X.25 communication option no longer available after June 2006

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FILE 'HOME' ENTERED AT 09:38:37 ON 07 JUN 2006

=> file reg
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                         0.21       0.21

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STRUCTURE FILE UPDATES:     6 JUN 2006  HIGHEST RN 887000-62-6
DICTIONARY FILE UPDATES:    6 JUN 2006  HIGHEST RN 887000-62-6

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TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

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*********************************************************************
*                                                                   *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005.  A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*                                                                   *
*********************************************************************

Structure search iteration limits have been increased.  See HELP SLIMITS
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REGISTRY includes numerically searchable data for experimental and
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experimental property data in the original document.  For information
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http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\107838013.str
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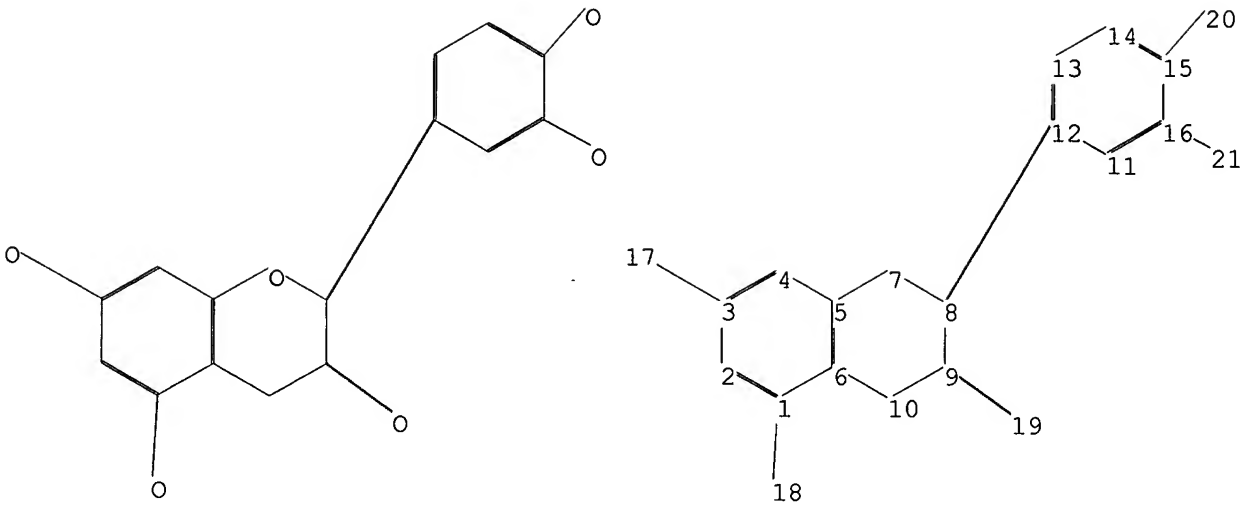

chain nodes :
17 18 19 20 21
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16
chain bonds :
1-18 3-17 8-12 9-19 15-20 16-21
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 11-12 11-16 12-13 13-14
14-15 15-16
exact/norm bonds :
1-18 3-17 5-7 6-10 7-8 8-9 9-10 9-19 15-20 16-21
exact bonds :
8-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:CLASS
20:CLASS 21:CLASS

L1 STRUCTURE UPLOADED

=> s l1
SAMPLE SEARCH INITIATED 09:39:16 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1036 TO ITERATE

100.0% PROCESSED 1036 ITERATIONS 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

```
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         18789 TO    22651
PROJECTED ANSWERS:             5639 TO     7841

L2           50 SEA SSS SAM L1

=> s l1 ful
FULL SEARCH INITIATED 09:39:24 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    20139 TO ITERATE

100.0% PROCESSED    20139 ITERATIONS                          6505 ANSWERS
SEARCH TIME: 00.00.01

L3          6505 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                              SINCE FILE      TOTAL
                                                      ENTRY    SESSION
FULL ESTIMATED COST                                  166.94     167.15

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FILE LAST UPDATED: 6 Jun 2006  (20060606/ED)

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=> s l3
L4        16900 L3

=> s l4 and (epicatechin or catechin)
           4775 EPICATECHIN
             63 EPICATECHINS
           4790 EPICATECHIN
                  (EPICATECHIN OR EPICATECHINS)
           8467 CATECHIN
           3106 CATECHINS
           9554 CATECHIN
                  (CATECHIN OR CATECHINS)
L5         8190 L4 AND (EPICATECHIN OR CATECHIN)

=> s l5 and dimer
         103875 DIMER
```
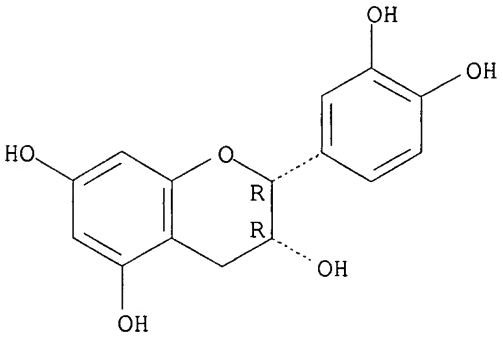

```
         59006 DIMERS
        136839 DIMER
                 (DIMER OR DIMERS)
L6         408 L5 AND DIMER

=> s l6 and (4,8)
       5339334 4
       2704086 8
        112120 4,8
                 (4(W)8)
L7          18 L6 AND (4,8)

=> s l5 and (process or make or made or prepar? or synthes? or method)
       2251291 PROCESS
       1525430 PROCESSES
       3360296 PROCESS
                 (PROCESS OR PROCESSES)
        231644 MAKE
        180294 MAKES
        399557 MAKE
                 (MAKE OR MAKES)
       1207430 MADE
            25 MADES
       1207451 MADE
                 (MADE OR MADES)
       1647869 PREPAR?
        122650 PREP
          2150 PREPS
        124594 PREP
                 (PREP OR PREPS)
       2008322 PREPD
            17 PREPDS
       2008334 PREPD
                 (PREPD OR PREPDS)
        121223 PREPG
            12 PREPGS
        121234 PREPG
                 (PREPG OR PREPGS)
       2711598 PREPN
        204470 PREPNS
       2865843 PREPN
                 (PREPN OR PREPNS)
       4743234 PREPAR?
                 (PREPAR? OR PREP OR PREPD OR PREPG OR PREPN)
       1535222 SYNTHES?
       3100220 METHOD
       1272104 METHODS
       4013969 METHOD
                 (METHOD OR METHODS)
L8         3366 L5 AND (PROCESS OR MAKE OR MADE OR PREPAR? OR SYNTHES? OR METHOD
                )

=> s l6 and (process or make or made or prepar? or synthes? or method)
       2251291 PROCESS
       1525430 PROCESSES
       3360296 PROCESS
                 (PROCESS OR PROCESSES)
        231644 MAKE
        180294 MAKES
        399557 MAKE
```

```
                (MAKE OR MAKES)
       1207430 MADE
            25 MADES
       1207451 MADE
                (MADE OR MADES)
       1647869 PREPAR?
        122650 PREP
          2150 PREPS
        124594 PREP
                (PREP OR PREPS)
       2008322 PREPD
            17 PREPDS
       2008334 PREPD
                (PREPD OR PREPDS)
        121223 PREPG
            12 PREPGS
        121234 PREPG
                (PREPG OR PREPGS)
       2711598 PREPN
        204470 PREPNS
       2865843 PREPN
                (PREPN OR PREPNS)
       4743234 PREPAR?
                (PREPAR? OR PREP OR PREPD OR PREPG OR PREPN)
       1535222 SYNTHES?
       3100220 METHOD
       1272104 METHODS
       4013969 METHOD
                (METHOD OR METHODS)
L9          185 L6 AND (PROCESS OR MAKE OR MADE OR PREPAR? OR SYNTHES? OR METHOD
                )

=> s l9 and (oxidation or oxidi?)
        433563 OXIDATION
          4850 OXIDATIONS
        434826 OXIDATION
                (OXIDATION OR OXIDATIONS)
        742953 OXIDN
          9337 OXIDNS
        744911 OXIDN
                (OXIDN OR OXIDNS)
        880077 OXIDATION
                (OXIDATION OR OXIDN)
        404853 OXIDI?
L10          27 L9 AND (OXIDATION OR OXIDI?)

=> d l10 ibib hitstr abs 1-27

L10  ANSWER 1 OF 27  CAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:         2005:1273656  CAPLUS
DOCUMENT NUMBER:          144:308365
TITLE:                    Transparent testa10 encodes a laccase-like enzyme
                          involved in oxidative polymerization of flavonoids in
                          Arabidopsis seed coat
AUTHOR(S):                Pourcel, Lucille; Routaboul, Jean-Marc; Kerhoas,
                          Lucien; Caboche, Michel; Lepiniec, Loic; Debeaujon,
                          Isabelle
CORPORATE SOURCE:         Laboratoire de Biologie des Semences, Unite Mixte de
                          Recherche 204, Institut National de la Recherche
                          Agronomique/Institut National Agronomique
```

Paris-Grignon, Institut Jean-Pierre Bourgin, Institut National de la Recherche Agronomique/Institut National Agronomique Paris-Grignon, Versailles, 78026, Fr.
SOURCE: Plant Cell (2005), 17(11), 2966-2980
CODEN: PLCEEW; ISSN: 1040-4651
PUBLISHER: American Society of Plant Biologists
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **490-46-0, Epicatechin**
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(transparent testa10 encodes laccase-like enzyme involved in oxidative polymerization of flavonoids in Arabidopsis seed coat)
RN 490-46-0 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



AB The Arabidopsis thaliana transparent testa10 (tt10) mutant exhibits a delay in developmentally determined browning of the seed coat, also called the testa. Seed coat browning is caused by the **oxidation** of flavonoids, particularly proanthocyanidins, which are polymers of flavan-3-ol subunits such as **epicatechin** and **catechin**. The tt10 mutant seeds accumulate more **epicatechin** monomers and more soluble proanthocyanidins than wild-type seeds. Moreover, intact testa cells of tt10 cannot trigger H2O2-independent browning in the presence of **epicatechin** and **catechin**, in contrast with wild-type cells. UV-visible light detection and mass spectrometry revealed that the major **oxidation** products obtained with **epicatechin** alone are yellow **dimers** called dehydrodiepicatechin A. These products differ from proanthocyanidins in the nature and position of their interflavan linkages. Flavonol composition was also affected in tt10 seeds, which exhibited a higher ratio of quercetin rhamnoside monomers vs. **dimers** than wild-type seeds. We identified the TT10 gene by a candidate gene approach. TT10 encodes a protein with strong similarity to laccase-like polyphenol oxidases. It is expressed essentially in developing testa, where it colocalizes with the flavonoid end products proanthocyanidins and flavonols. Together, these data establish that TT10 is involved in the oxidative polymerization of flavonoids and functions as a laccase-type flavonoid oxidase.

REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

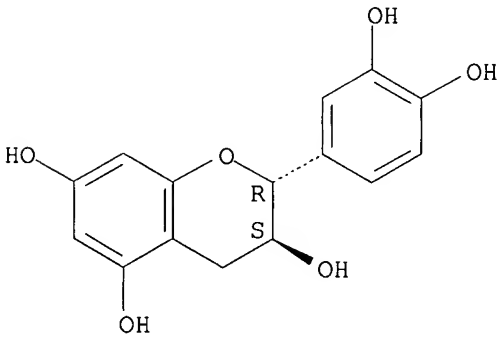
L10 ANSWER 2 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:1165929 CAPLUS
DOCUMENT NUMBER: 144:16442

TITLE: Phenolics as potential antioxidant therapeutic agents: Mechanism and actions
AUTHOR(S): Soobrattee, M. A.; Neergheen, V. S.; Luximon-Ramma, A.; Aruoma, O. I.; Bahorun, T.
CORPORATE SOURCE: Department of Biosciences, Faculty of Science, University of Mauritius, Reduit, Mauritius
SOURCE: Mutation Research (2005), 579(1-2), 200-213
CODEN: MUREAV; ISSN: 0027-5107
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **154-23-4**, (+)-**Catechin 490-46-0**, (-)-**Epicatechin 528-58-5**, Cyanidin chloride **970-74-1**, (-)-Epigallocatechin **989-51-5**, (-)-Epigallocatechin gallate **1257-08-5 20315-25-7**, Procyanidin B1 **29106-49-8**, Procyanidin B2
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(phenolics as potential antioxidant therapeutic agents and mechanism and actions)

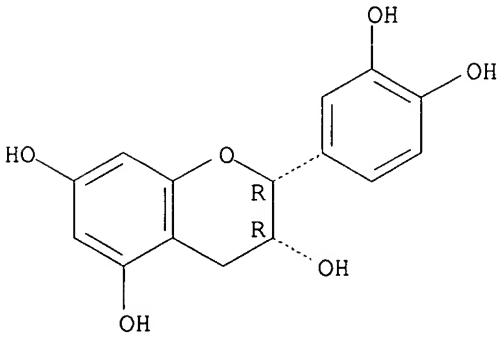
RN 154-23-4 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

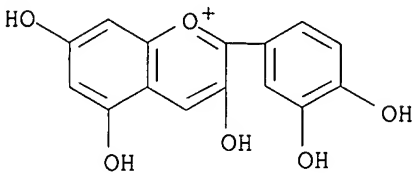


RN 490-46-0 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



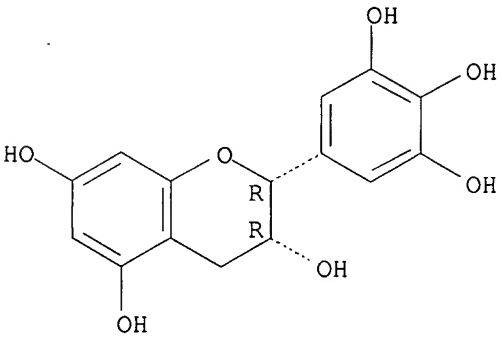
RN 528-58-5 CAPLUS
CN 1-Benzopyrylium, 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-, chloride (9CI) (CA INDEX NAME)



● Cl^-

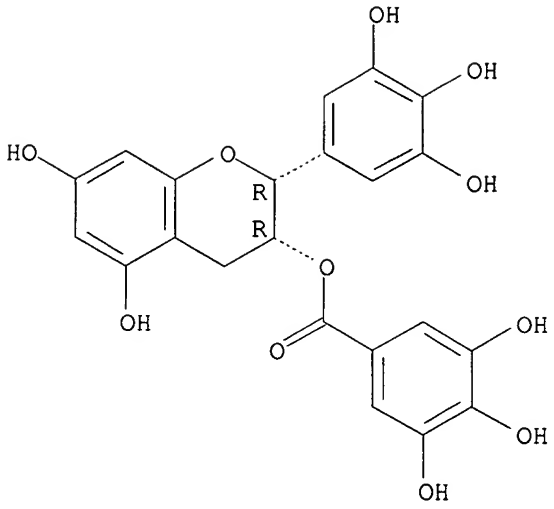
RN 970-74-1 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 3,4-dihydro-2-(3,4,5-trihydroxyphenyl)-, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



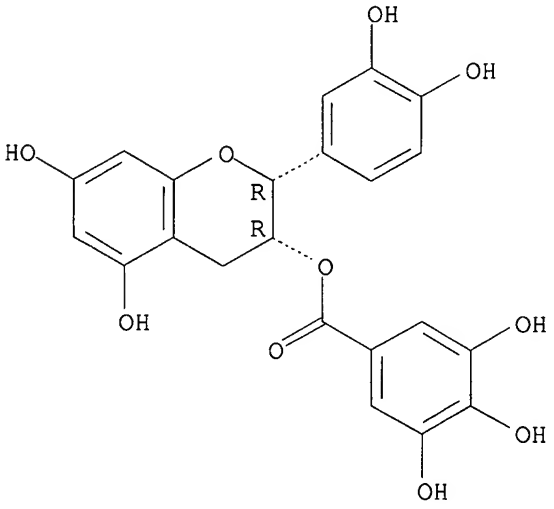
RN 989-51-5 CAPLUS
CN Benzoic acid, 3,4,5-trihydroxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



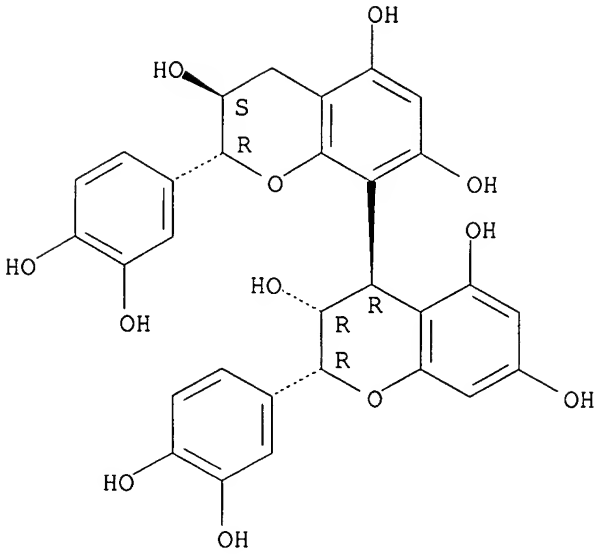
RN 1257-08-5 CAPLUS
CN Benzoic acid, 3,4,5-trihydroxy-, (2R,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



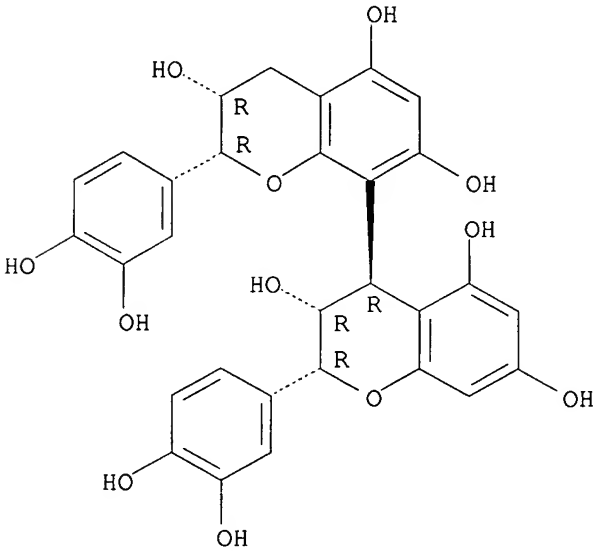
RN 20315-25-7 CAPLUS
CN [4,8'-Bi-2H-1-benzopyran]-3,3',5,5',7,7'-hexol, 2,2'-bis(3,4-dihydroxyphenyl)-3,3',4,4'-tetrahydro-, (2R,2'R,3R,3'S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 29106-49-8 CAPLUS
CN [4,8'-Bi-2H-1-benzopyran]-3,3',5,5',7,7'-hexol, 2,2'-bis(3,4-dihydroxyphenyl)-3,3',4,4'-tetrahydro-, (2R,2'R,3R,3'R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

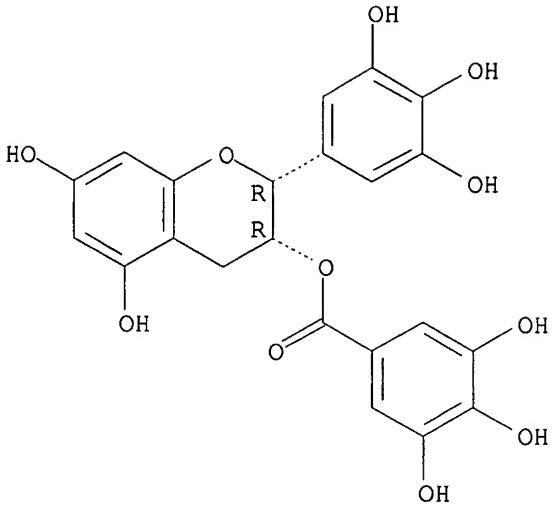


AB Accumulating chemical, biochem., clin. and epidemiol. evidence supports the chemoprotective effects of phenolic antioxidants against oxidative stress-mediated disorders. The pharmacol. actions of phenolic antioxidants stem mainly from their free radical scavenging and metal chelating properties as well as their effects on cell signaling pathways and on gene expression. The antioxidant capacities of phenolic compds. that are widely distributed in plant-based diets were assessed by the Trolox equivalent antioxidant capacity (TEAC), the ferric reducing antioxidant

power (FRAP), the hypochlorite scavenging capacity, the deoxyribose **method** and the copper-phenanthroline-dependent DNA **oxidn** . assays. Based on the TEAC, FRAP and hypochlorite scavenging data, the observed activity order was: procyanidin **dimer** > flavanol > flavonol > hydroxycinnamic acids > simple phenolic acids. Among the flavonol aglycons, the antioxidant propensities decrease in the order quercetin, myricetin and kaempferol. Gallic acid and rosmarinic acid were the most potent antioxidants among the simple phenolic and hydroxycinnamic acids, resp. Ferulic acid displayed the highest inhibitory activity against deoxyribose degradation but no structure-activity relation could be established for the activities of the phenolic compds. in the deoxyribose assay. The efficacies of the phenolic compds. differ depending on the mechanism of antioxidant action in the resp. assay used, with procyanidin **dimers** and flavan-3-ols showing very potent activities in most of the systems tested. Compared to the physiol. active (glutathione, α-tocopherol, ergothioneine) and synthetic (Trolox, BHA, BHT) antioxidants, these compds. exhibited much higher efficacy. Plant-derived phenolics represents good sources of natural antioxidants, however, further investigation on the mol. mechanism of action of these phytochems. is crucial to the evaluation of their potential as prophylactic agents.
REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

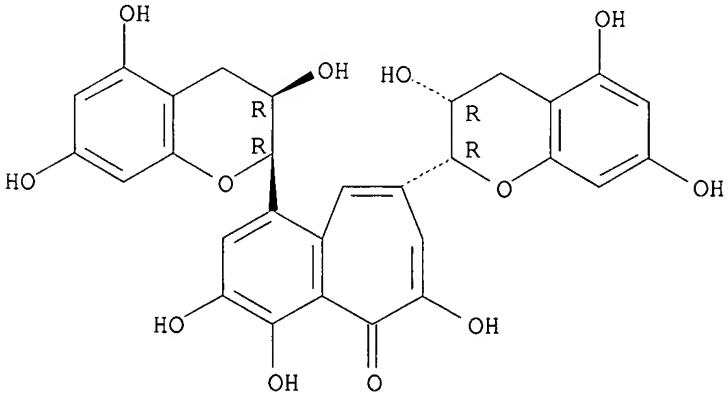
L10 ANSWER 3 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:904441 CAPLUS
DOCUMENT NUMBER: 143:404966
TITLE: A novel black tea pigment and two new **oxidation** products of epigallocatechin-3-O-gallate
AUTHOR(S): Tanaka, Takashi; Matsuo, Yosuke; Kouno, Isao
CORPORATE SOURCE: Graduate School of Biomedical Sciences, Nagasaki University, Nagasaki, 852-8521, Japan
SOURCE: Journal of Agricultural and Food Chemistry (2005), 53(19), 7571-7578
CODEN: JAFCAU; ISSN: 0021-8561
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **989-51-5**, Epigallocatechin-3-O-gallate **4670-05-7D**, Theaflavin, derivs. **89064-31-3**, Theasinensin A **867278-31-7 867358-20-1**, Dehydrotheasinensin AQ
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(black tea pigment and two new **oxidation** products of epigallocatechin-3-O-gallate)
RN 989-51-5 CAPLUS
CN Benzoic acid, 3,4,5-trihydroxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



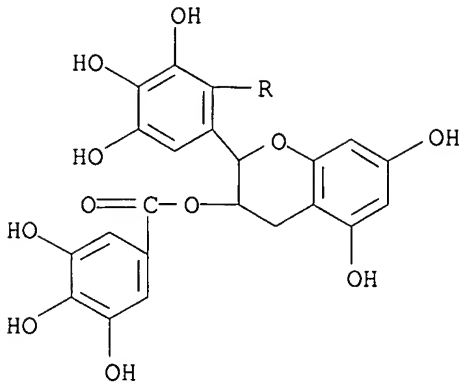
RN 4670-05-7 CAPLUS
CN 5H-Benzocyclohepten-5-one, 1,8-bis[(2R,3R)-3,4-dihydro-3,5,7-trihydroxy-2H-1-benzopyran-2-yl]-3,4,6-trihydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

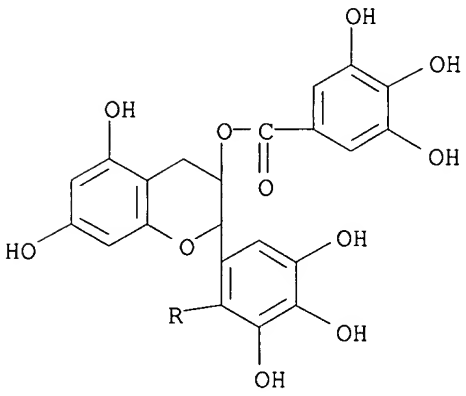


RN 89064-31-3 CAPLUS
CN Benzoic acid, 3,4,5-trihydroxy-, [(1R)-4,4',5,5',6,6'-hexahydroxy[1,1'-biphenyl]-2,2'-diyl]bis[(2R,3R)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-2,3-diyl] ester (9CI) (CA INDEX NAME)

PAGE 1-A



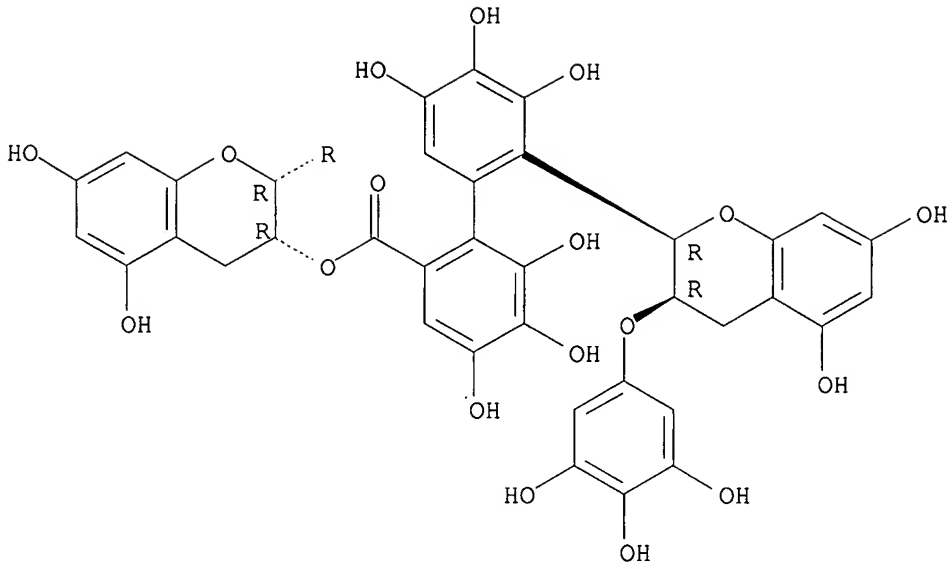
PAGE 2-A



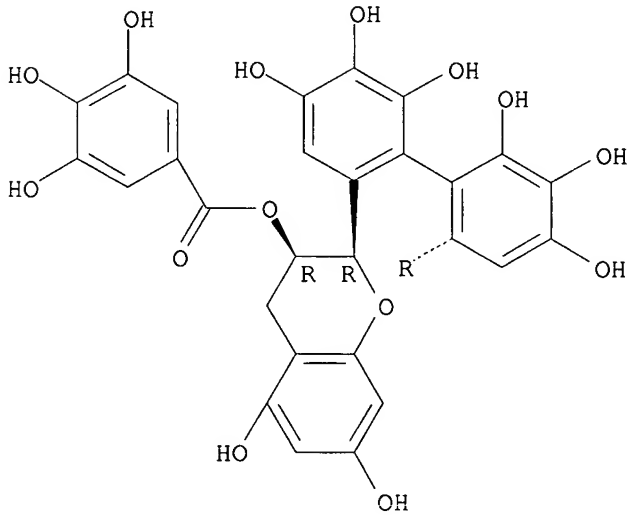
RN 867278-31-7 CAPLUS
CN [1,1'-Biphenyl]-2-carboxylic acid, 2'-[(2R,3R)-3,4-dihydro-5,7-dihydroxy-3-(3,4,5-trihydroxyphenoxy)-2H-1-benzopyran-2-yl]-3',4,4',5,5',6-hexahydroxy-, (2R,3R)-2-[6'-[(2R,3R)-3,4-dihydro-5,7-dihydroxy-3-[(3,4,5-trihydroxybenzoyl)oxy]-2H-1-benzopyran-2-yl]-2',3',4,4',5,6-hexahydroxy[1,1'-biphenyl]-2-yl]-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



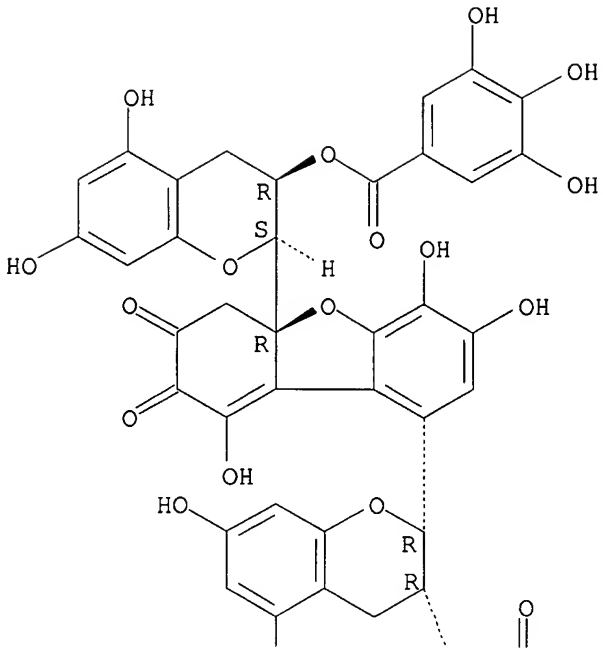
PAGE 2-A



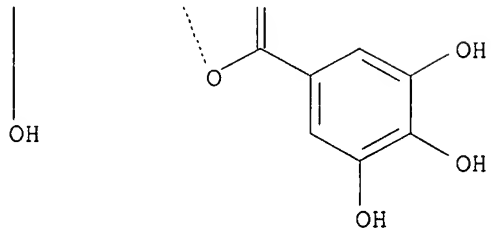
RN 867358-20-1 CAPLUS
CN Benzoic acid, 3,4,5-trihydroxy-, (7,8-dihydro-3,4,9-trihydroxy-7,8-dioxo-1,5a(6H)-dibenzofurandiyl)bis(3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-2,3-diyl) ester, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

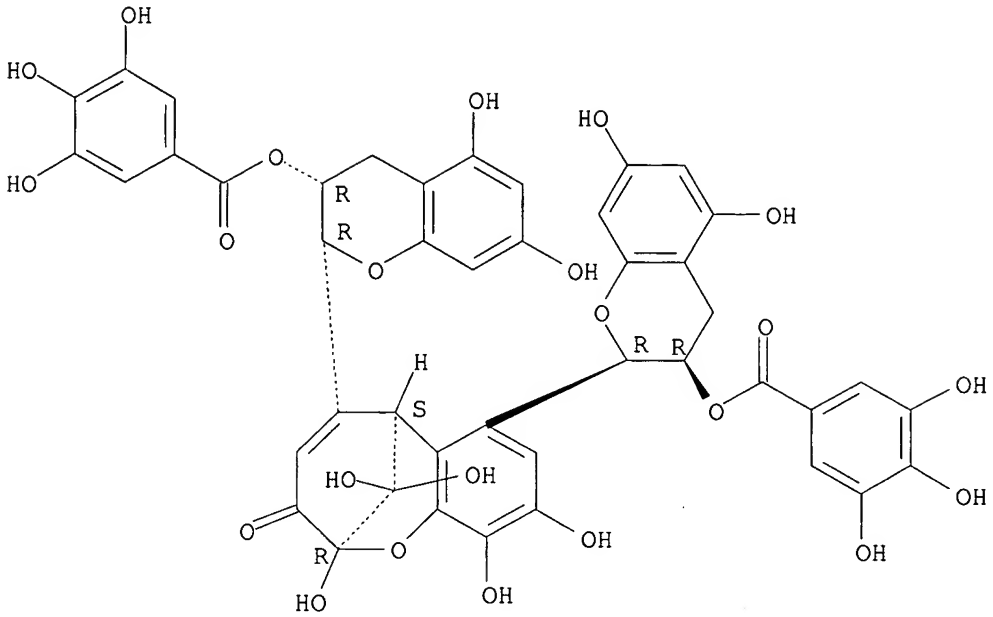


IT **625371-09-7**, Dehydrotheasinensin A
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(black tea pigment and two new **oxidation** products of epigallocatechin-3-O-gallate)

RN 625371-09-7 CAPLUS

CN Benzoic acid, 3,4,5-trihydroxy-, [(2R,6S)-3,6-dihydro-2,9,10,11,11-pentahydroxy-3-oxo-2,6-methano-2H-1-benzoxocin-5,7-diyl]bis[(2R,3R)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-2,3-diyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



AB During tea fermentation, **oxidation**-reduction dismutation of a number of quinone metabolites of tea **catechins** yields numerous minor products, which **make** it difficult to sep. and purify black tea polyphenols. In this study, epigallocatechin-3-O-gallate was enzymically **oxidized** and then the unstable quinone metabolites in the **oxidation** mixture were hydrogenated with 2-mercaptoethanol to reduce production of inseparable minor dismutation products. As a result, three new **oxidation** products including a new black tea pigment were isolated, and their structures were determined based on chemical and spectroscopic data. Dehydrotheasinensin AQ is a new reddish-orange pigment with a 1,2-diketone structure, and its presence in com. black tea was confirmed. In addition, a new quinone **dimer** with a complex caged structure and a trimer of epigallocatechin-3-O-gallate were also isolated and their production mechanisms are proposed. The presence of this trimer suggested participation of galloyl quinones in production of minor polyphenols in black tea.

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

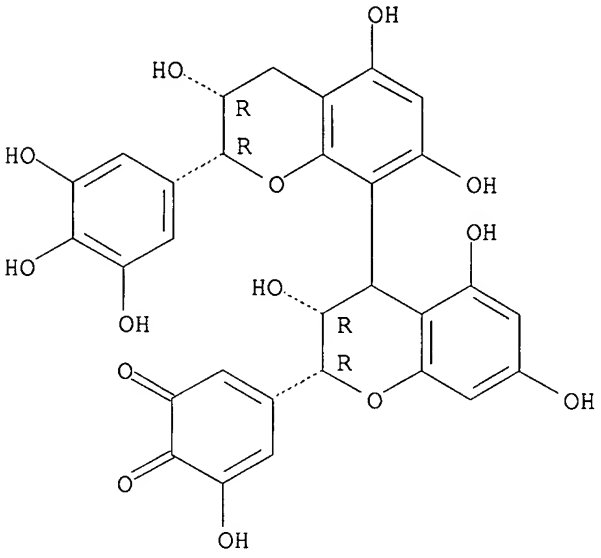
L10 ANSWER 4 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:513695 CAPLUS
DOCUMENT NUMBER: 141:410544
TITLE: Study of the **oxidation processes** of **catechins** by on-line electrolysis/ESI/MS
AUTHOR(S): Yamaguchi, Masashi; Mizooku, Yasuo; Osakai, Toshiyuki; Kimoto, Takashi; Arakawa, Ryuichi
CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering, Kansai University, Suita-shi, Osaka, 564-8680, Japan
SOURCE: Bunseki Kagaku (2004), 53(6), 547-553
CODEN: BNSKAK; ISSN: 0525-1931
PUBLISHER: Nippon Bunseki Kagakkai
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
IT **791816-85-8**

RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)
(**oxidation** of **catechins** examined by online electrolysis/ESI/MS)

RN 791816-85-8 CAPLUS

CN 3,5-Cyclohexadiene-1,2-dione, 3-hydroxy-5-[(2R,2'R,3R,3'R)-3,3',4,4'-tetrahydro-3,3',5,5',7,7'-hexahydroxy-2'-(3,4,5-trihydroxyphenyl)[4,8'-bi-2H-1-benzopyran]-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

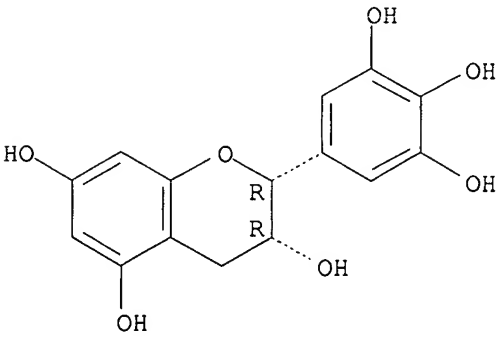


IT **970-74-1**, (-)-Epigallocatechin **989-51-5**, (-)-Epigallocatechin gallate **1257-08-5**
RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)
(**oxidation** of **catechins** examined by online electrolysis/ESI/MS)

RN 970-74-1 CAPLUS

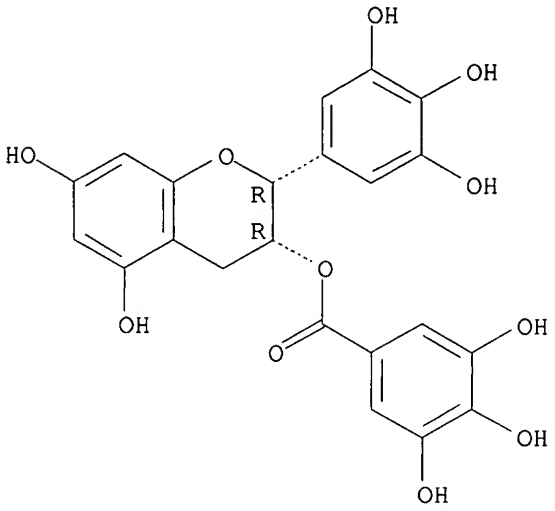
CN 2H-1-Benzopyran-3,5,7-triol, 3,4-dihydro-2-(3,4,5-trihydroxyphenyl)-, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



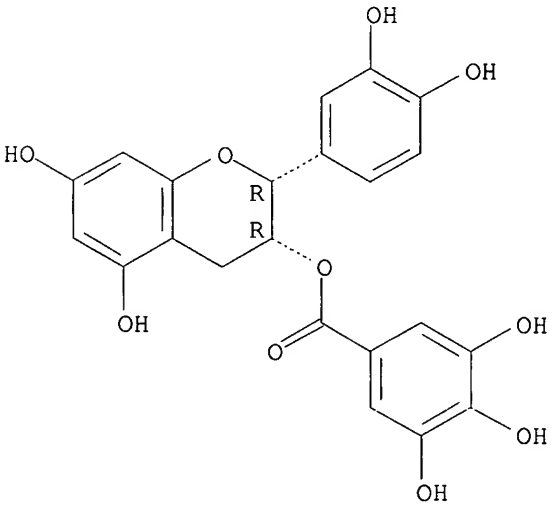
RN 989-51-5 CAPLUS
CN Benzoic acid, 3,4,5-trihydroxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 1257-08-5 CAPLUS
CN Benzoic acid, 3,4,5-trihydroxy-, (2R,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

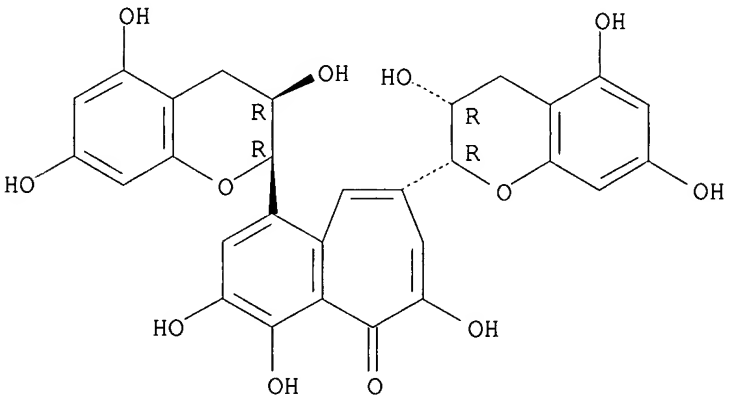


AB Much attention was focused on the strong antioxidant activity and antitumorigenic property of **catechins** extracted from green tea. However, not many studies on the **oxidation process** of **catechins** were conducted. The authors employed an online electrochem./electrospray ionization mass spectrometry (EC/ESI-MS) technique to identify unstable **oxidation** products of **catechins**. The authors have succeeded in detecting **dimer**

products formed by the electrolysis of (-)-epigallocatechin, (-)-**epicatechin** gallate and (-)-epigallocatechin gallate. EC/ESI-MS was a useful technique to study electrochem. **oxidation process** of antioxidants.

L10 ANSWER 5 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:690290 CAPLUS
DOCUMENT NUMBER: 139:337052
TITLE: **Oxidation** of tea **catechins**: chemical structures and reaction mechanism
AUTHOR(S): Tanaka, Takashi; Kouno, Isao
CORPORATE SOURCE: Department of Molecular Medicinal Sciences, Graduate School of Biomedical Sciences, Nagasaki University, Nagasaki, 852-8521, Japan
SOURCE: Food Science and Technology Research (2003), 9(2), 128-133
CODEN: FSTRFS; ISSN: 1344-6606
PUBLISHER: Japanese Society for Food Science and Technology
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
IT **4670-05-7**, Theaflavin
RL: BCP (Biochemical process); BIOL (Biological study); PROC (Process)
(**oxidation** of tea **catechins** related to polyphenols in black tea)
RN 4670-05-7 CAPLUS
CN 5H-Benzocyclohepten-5-one, 1,8-bis[(2R,3R)-3,4-dihydro-3,5,7-trihydroxy-2H-1-benzopyran-2-yl]-3,4,6-trihydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



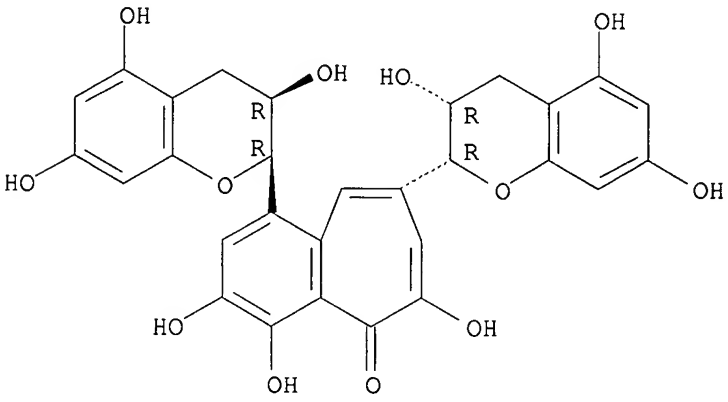
AB A review. Black tea accounts for almost 80% of the world's tea production and is the most important source of polyphenol in the world. However, little has been known about the chemical of black tea polyphenols due to their complexity. Since most of the black tea polyphenols are produced by enzymic **oxidation** of green tea **catechins**, in vitro model fermentation expts. using purified **catechins** are very useful, and recently structures of some novel **oxidation** products of theaflavins, black tea pigments, have been elucidated. In addition, accumulation of unstable **dimer** quinones of epigallocatechin and its gallate during tea fermentation has been demonstrated, and the **dimer** quinones are converted to theasinensins, another major polyphenol characteristic of black tea, on heating. Formation and degradation of theaflavins and epigallocatechin **dimer** quinones are major pathways in **catechin oxidation** during tea fermentation and

understanding the chemical mechanism is important in clarifying black tea polyphenols.

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

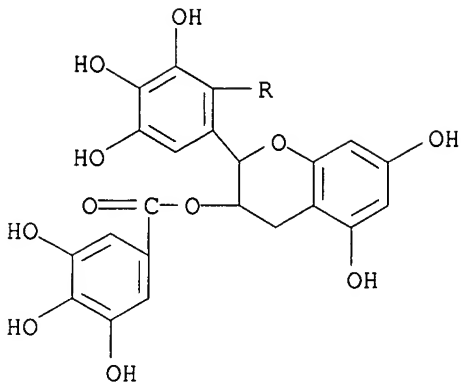
L10 ANSWER 6 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:613003 CAPLUS
DOCUMENT NUMBER: 139:393356
TITLE: **Oxidation** mechanism of **catechins** and related polyphenols
AUTHOR(S): Tanaka, Takashi; Mine, Chie; Matsuda, Miyuki; Inoue, Kyoko; Kouno, Isao
CORPORATE SOURCE: School of Pharmaceutical Sciences, Nagasaki University, Japan
SOURCE: Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (2001), 43rd, 329-334
CODEN: TYKYDS
PUBLISHER: Nippon Kagakkai
DOCUMENT TYPE: Journal; General Review
LANGUAGE: Japanese
IT **4670-05-7**, Theaflavin **89064-31-3**, Theasinensin A
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(**oxidation** mechanism of **catechins** and related polyphenols)
RN 4670-05-7 CAPLUS
CN 5H-Benzocyclohepten-5-one, 1,8-bis[(2R,3R)-3,4-dihydro-3,5,7-trihydroxy-2H-1-benzopyran-2-yl]-3,4,6-trihydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

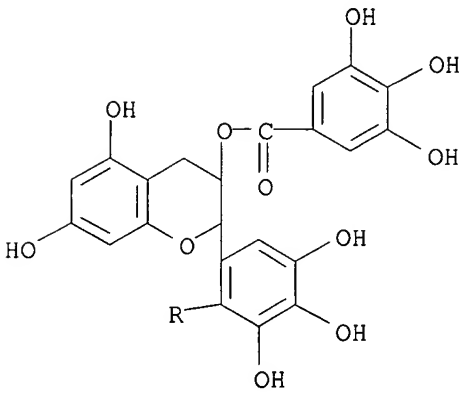


RN 89064-31-3 CAPLUS
CN Benzoic acid, 3,4,5-trihydroxy-, [(1R)-4,4',5,5',6,6'-hexahydroxy[1,1'-biphenyl]-2,2'-diyl]bis[(2R,3R)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-2,3-diyl] ester (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

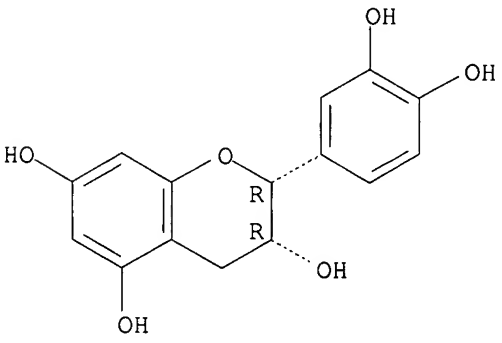


AB A review. **Oxidation** of green tea **catechins** under various conditions was chemical investigated. When a mixture of (-)-**epicatechin** (EC) and (-)-epigallocatechin (EGCG) was treated with homogenate of fresh tea leaves, theasinensin A and a new dimeric product 1, derived by Diels-Alder coupling of EGCG with its **oxidation** product, were obtained. On the other hand, auto-**oxidation** of theaflavin (TF) at pH 7.3 gave theanaphthoquinone (TNQ) and a new flavan-3-of tetramer (2) having a bicyclooctane skeleton, which was also a Diels-Alder product of dehydro-TF and dihydro-TNQ. The results suggested that formation of quinehydrone type n-n complexes is important in the **catechin oxidation** In the **process** of TF production from EC and (-)-epigallocatechin (EGC) by banana polyphenoloxidase, EC was rapidly **oxidized** to EC-quinone and the resulting EC-quinone **oxidized** EGC to EGC-quinone. After EGC was completely consumed, the EC-quinone began to **oxidize** TF to TNQ. This coupled **oxidation** mechanism was shown by rapid decrease of EGC in the presence of EC and the sparing of EC at the beginning of the reaction. In addition, when the reaction was conducted in the presence of glutathione, about 80% of EGC was not **oxidized**, even though EC was completely converted to its glutathione conjugates. Furthermore, it was also suggested that theasinensins (TS), **dimers** of EGC or EGCG found in black tea, were generated by reduction of corresponding quinones

(TS-quinones) formed by stereospecific coupling of two EGC-quinones. The presence of TS-quinones in the homogenate of fresh tea leaves was also confirmed by isolation of their phenazine derivs. These results suggested that thearubigins, the uncharacterized heterogeneous polymer of black tea, are probably produced by polymerization the quinones derived from **catechins** and their metabolites during tea fermentation

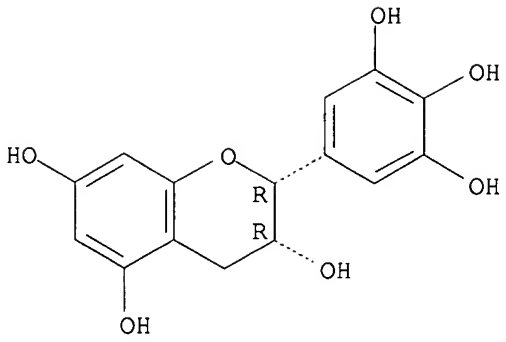
L10 ANSWER 7 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:831351 CAPLUS
DOCUMENT NUMBER: 138:72278
TITLE: Structures of two new **oxidation** products of green tea polyphenols generated by model tea fermentation
AUTHOR(S): Tanaka, Takashi; Mine, Chie; Kouno, Isao
CORPORATE SOURCE: Graduate School of Biomedical Sciences, Department of Molecular Medicinal Sciences, Nagasaki University, Nagasaki, 852-8521, Japan
SOURCE: Tetrahedron (2002), 58(43), 8851-8856
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **490-46-0**, (-)-**Epicatechin 970-74-1**, (-)-Epigallocatechin **989-51-5**, (-)-Epigallocatechin 3-O-gallate
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(structures of two new **oxidation** products of green tea polyphenols generated by model tea fermentation)
RN 490-46-0 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



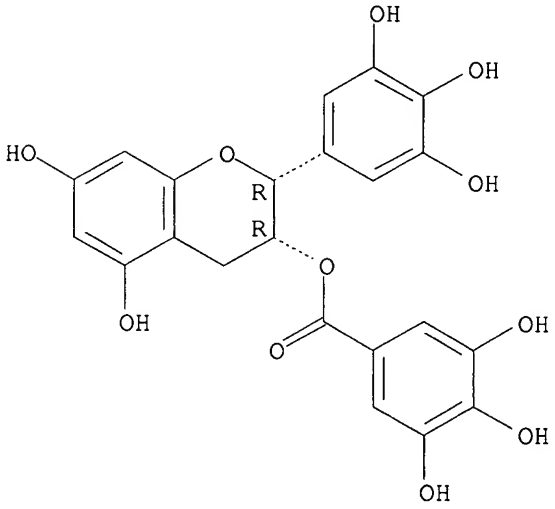
RN 970-74-1 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 3,4-dihydro-2-(3,4,5-trihydroxyphenyl)-, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



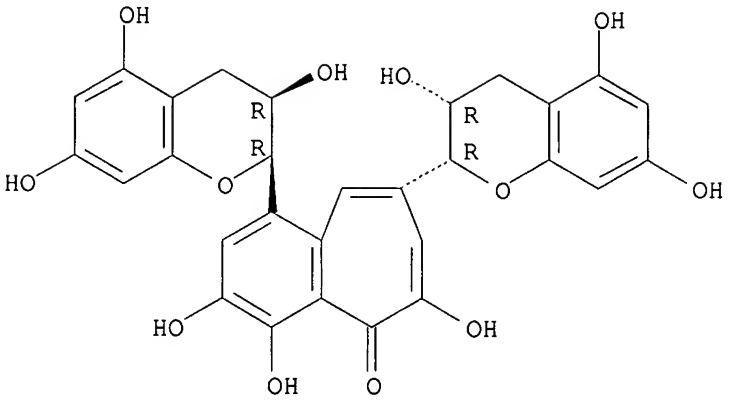
RN 989-51-5 CAPLUS
CN Benzoic acid, 3,4,5-trihydroxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT **4670-05-7**, Theaflavin
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
(structures of two new **oxidation** products of green tea polyphenols generated by model tea fermentation)
RN 4670-05-7 CAPLUS
CN 5H-Benzocyclohepten-5-one, 1,8-bis[(2R,3R)-3,4-dihydro-3,5,7-trihydroxy-2H-1-benzopyran-2-yl]-3,4,6-trihydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



AB To clarify the **oxidation** mechanism of green tea **catechins** during tea fermentation, pure **catechins** were **oxidized** with a **catechin**-free homogenate of tea leaf. **Oxidation** of a mixture of (-)-**epicatechin** and (-)-epigallocatechin yielded a new metabolite, named dehydrotheaflavin, produced by the **oxidation** of a benzotropolone moiety of the black tea pigment theaflavin. Similar **oxidation** of a mixture of (-)-**epicatechin** and (-)-epigallocatechin 3-O-gallate afforded a new **dimer** of (-)-epigallocatechin 3-O-gallate, which was generated by the **oxidn**. and cycloaddn. of two pyrogallol rings. Structures were determined by spectroscopic **method**, and the **oxidation** mechanisms for the formation of the products were proposed.

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 8 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:185102 CAPLUS
DOCUMENT NUMBER: 136:247439
TITLE: **Process** for **preparing** 4α-aryl substituted **epicatechin** derivatives
INVENTOR(S): Kozikowski, Alan P.; Romanczyk, Leo J., Jr.; Tueckmantel, Werner
PATENT ASSIGNEE(S): Mars, Inc., USA
SOURCE: PCT Int. Appl., 31 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002020506	A2	20020314	WO 2001-US26175	20010821
WO 2002020506	A3	20030206		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,

BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 6476241	B1	20021105	US 2000-655360		20000905
CA 2421513	AA	20020314	CA 2001-2421513		20010821
AU 2001083472	A5	20020322	AU 2001-83472		20010821
EP 1317437	A2	20030611	EP 2001-962277		20010821
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
JP 2004508362	T2	20040318	JP 2002-525127		20010821
US 2003100775	A1	20030529	US 2002-214830		20020808
US 6720432	B2	20040413			
US 2005014958	A1	20050120	US 2004-783801		20040220
PRIORITY APPLN. INFO.:			US 2000-655360	A	20000905
			WO 2001-US26175	W	20010821
			US 2002-214830	A3	20020808

OTHER SOURCE(S): CASREACT 136:247439; MARPAT 136:247439

IT **89385-19-3P 223387-39-1P 299412-40-1P**
301539-02-6P 330936-12-4P 330936-13-5P
330936-15-7P 330936-17-9P 330936-23-7P
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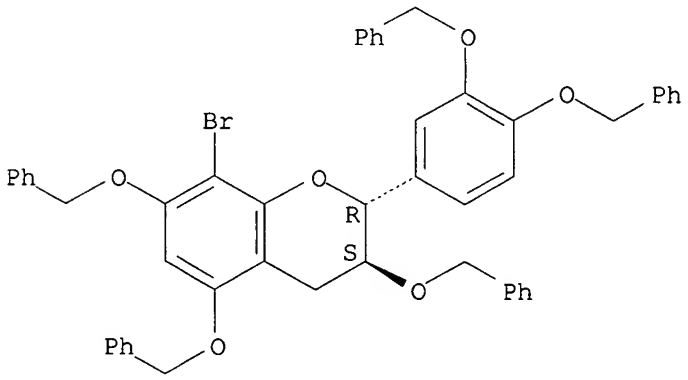
330936-27-1P 330936-28-2P 330936-30-6P
330936-31-7P 403651-95-6P 403651-96-7P
403820-84-8P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(**methods** for the **preparation** of 4α-aryl substituted **epicatechin** derivs.)

RN 89385-19-3 CAPLUS

CN 2H-1-Benzopyran, 2-[3,4-bis(phenylmethoxy)phenyl]-8-bromo-3,4-dihydro-3,5,7-tris(phenylmethoxy)-, (2R,3S)- (9CI) (CA INDEX NAME)

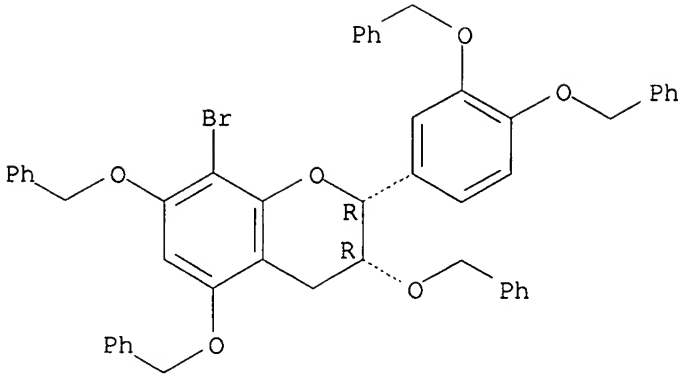
Absolute stereochemistry. Rotation (-).



RN 223387-39-1 CAPLUS

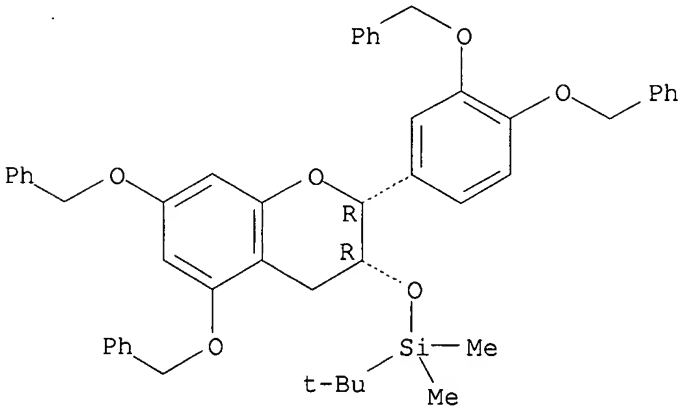
CN 2H-1-Benzopyran, 2-[3,4-bis(phenylmethoxy)phenyl]-8-bromo-3,4-dihydro-3,5,7-tris(phenylmethoxy)-, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



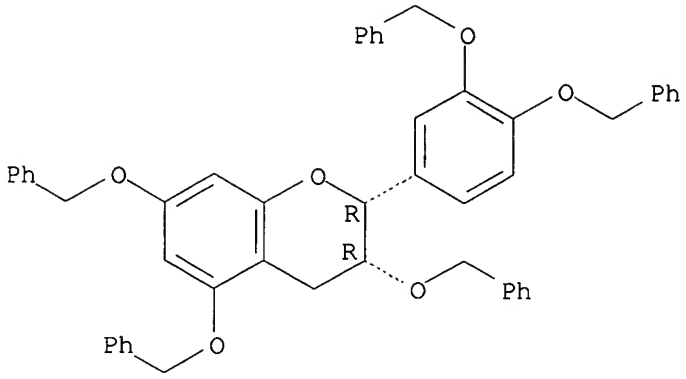
RN 299412-40-1 CAPLUS
CN Silane, [[(2R,3R)-2-[3,4-bis(phenylmethoxy)phenyl]-3,4-dihydro-5,7-bis(phenylmethoxy)-2H-1-benzopyran-3-yl]oxy](1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



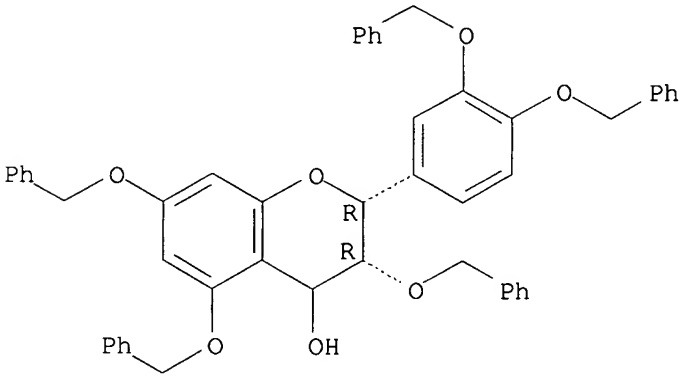
RN 301539-02-6 CAPLUS
CN 2H-1-Benzopyran, 2-[3,4-bis(phenylmethoxy)phenyl]-3,4-dihydro-3,5,7-tris(phenylmethoxy)-, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



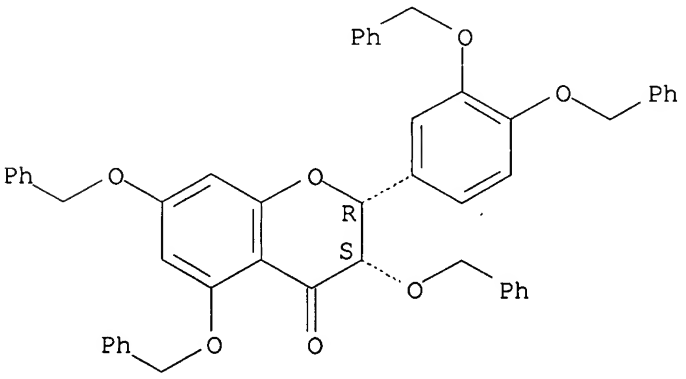
RN 330936-12-4 CAPLUS
CN 2H-1-Benzopyran-4-ol, 2-[3,4-bis(phenylmethoxy)phenyl]-3,4-dihydro-3,5,7-tris(phenylmethoxy)-, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



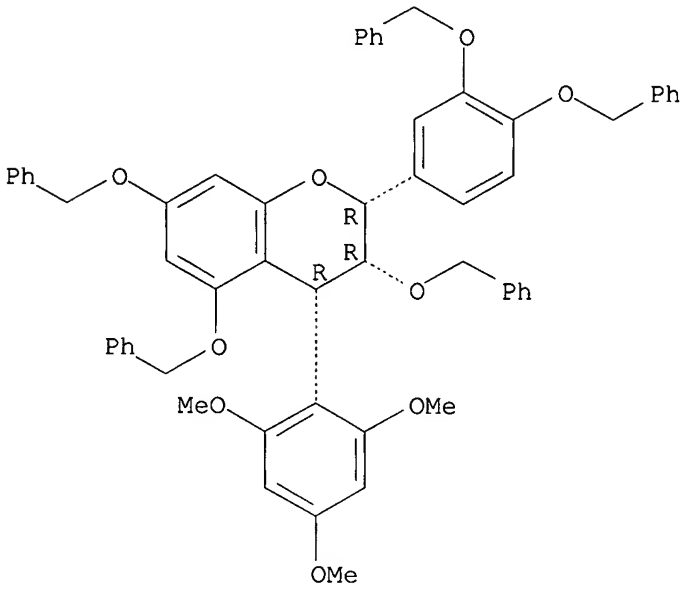
RN 330936-13-5 CAPLUS
CN 4H-1-Benzopyran-4-one, 2-[3,4-bis(phenylmethoxy)phenyl]-2,3-dihydro-3,5,7-tris(phenylmethoxy)-, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



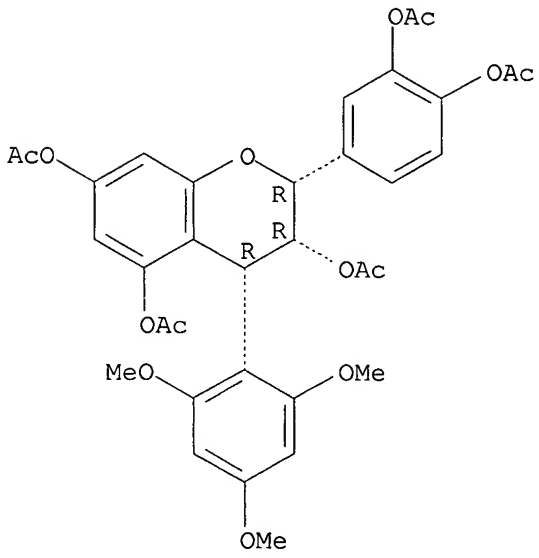
RN 330936-15-7 CAPLUS
CN 2H-1-Benzopyran, 2-[3,4-bis(phenylmethoxy)phenyl]-3,4-dihydro-3,5,7-tris(phenylmethoxy)-4-(2,4,6-trimethoxyphenyl)-, (2R,3R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 330936-17-9 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 2-[3,4-bis(acetyloxy)phenyl]-3,4-dihydro-4-(2,4,6-trimethoxyphenyl)-, triacetate, (2R,3R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

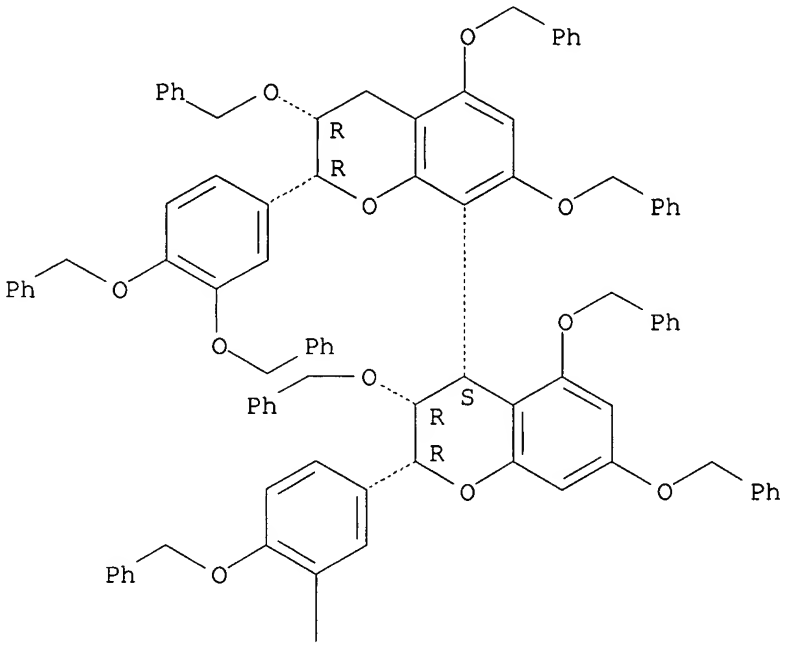


RN 330936-23-7 CAPLUS

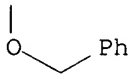
CN 4,8'-Bi-2H-1-benzopyran, 2,2'-bis[3,4-bis(phenylmethoxy)phenyl]-3,3',4,4'-tetrahydro-3,3',5,5',7,7'-hexakis(phenylmethoxy)-, (2R,2'R,3R,3'R,4S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



PAGE 2-A

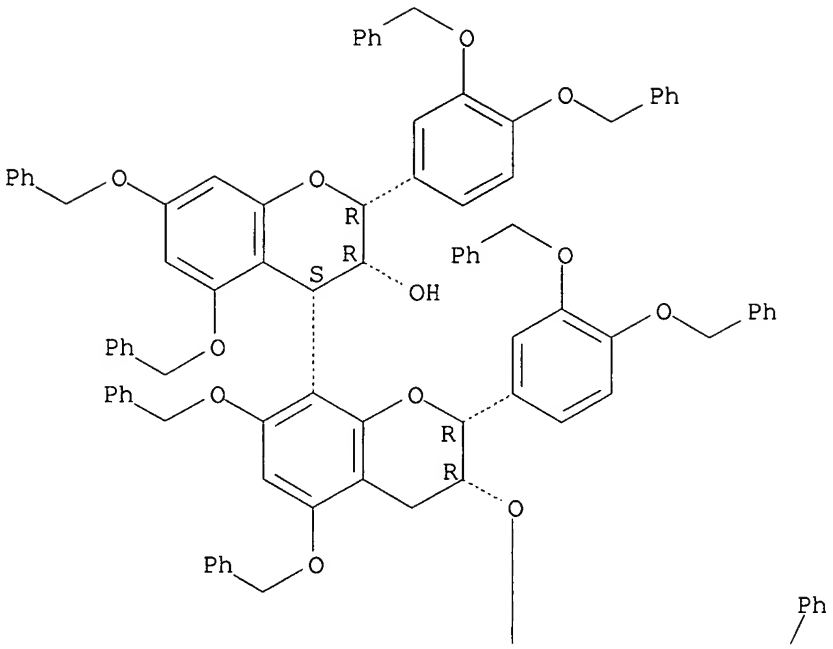


RN 330936-24-8 CAPLUS

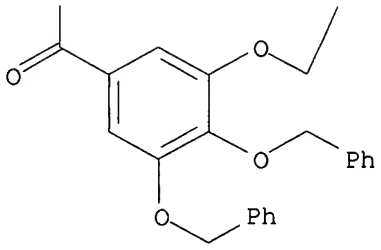
CN Benzoic acid, 3,4,5-tris(phenylmethoxy)-, (2R,2'R,3R,3'R,4S)-2,2'-bis[3,4-bis(phenylmethoxy)phenyl]-3,3',4,4'-tetrahydro-3-hydroxy-5,5',7,7'-tetrakis(phenylmethoxy)[4,8'-bi-2H-1-benzopyran]-3'-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



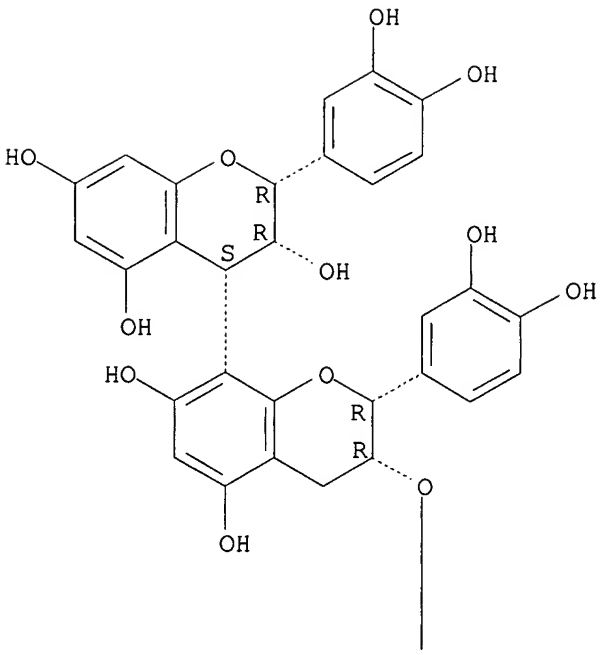
PAGE 2-A



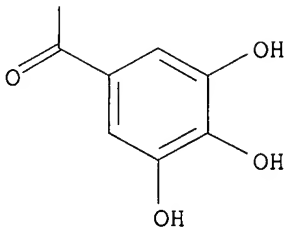
RN 330936-25-9 CAPLUS
CN Benzoic acid, 3,4,5-trihydroxy-, (2R,2'R,3R,3'R,4S)-2,2'-bis(3,4-dihydroxyphenyl)-3,3',4,4'-tetrahydro-3,5,5',7,7'-pentahydroxy[4,8'-bi-2H-1-benzopyran]-3'-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

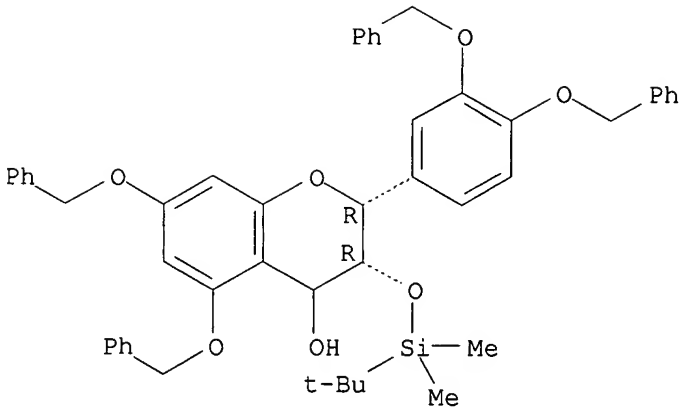


PAGE 2-A



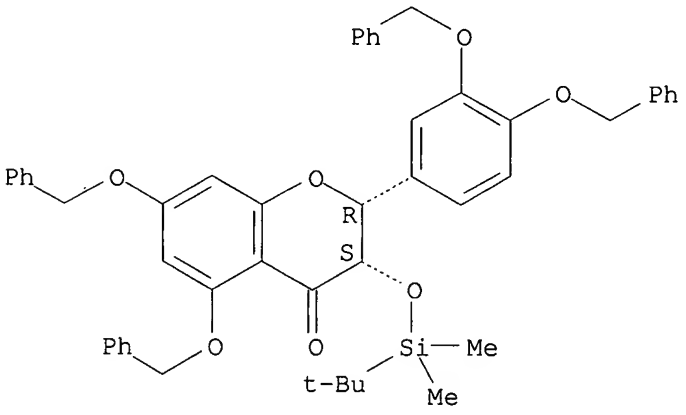
RN 330936-26-0 CAPLUS
CN 2H-1-Benzopyran-4-ol, 2-[3,4-bis(phenylmethoxy)phenyl]-3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-3,4-dihydro-5,7-bis(phenylmethoxy)-, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



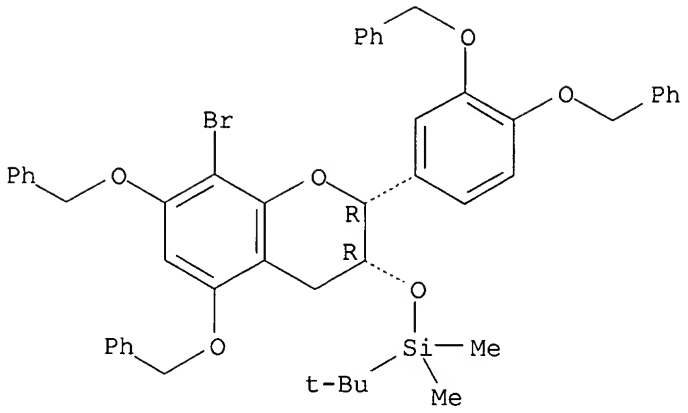
RN 330936-27-1 CAPLUS
CN 4H-1-Benzopyran-4-one, 2-[3,4-bis(phenylmethoxy)phenyl]-3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2,3-dihydro-5,7-bis(phenylmethoxy)-, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 330936-28-2 CAPLUS
CN Silane, [[(2R,3R)-2-[3,4-bis(phenylmethoxy)phenyl]-8-bromo-3,4-dihydro-5,7-bis(phenylmethoxy)-2H-1-benzopyran-3-yl]oxy](1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)

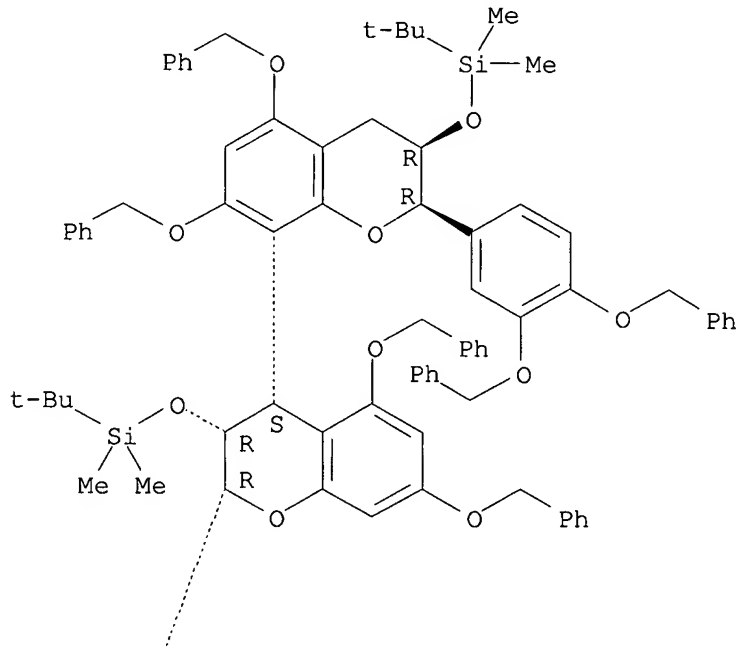
Absolute stereochemistry.



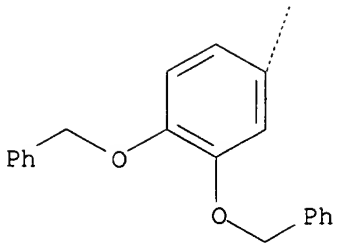
RN 330936-30-6 CAPLUS
CN Silane, [[(2R,2'R,3R,3'R,4S)-2,2'-bis[3,4-bis(phenylmethoxy)phenyl]-3,3',4,4'-tetrahydro-5,7-bis(phenylmethoxy)[4,8'-bi-2H-1-benzopyran]-3,3'-diyl]bis(oxy)]bis[(1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A

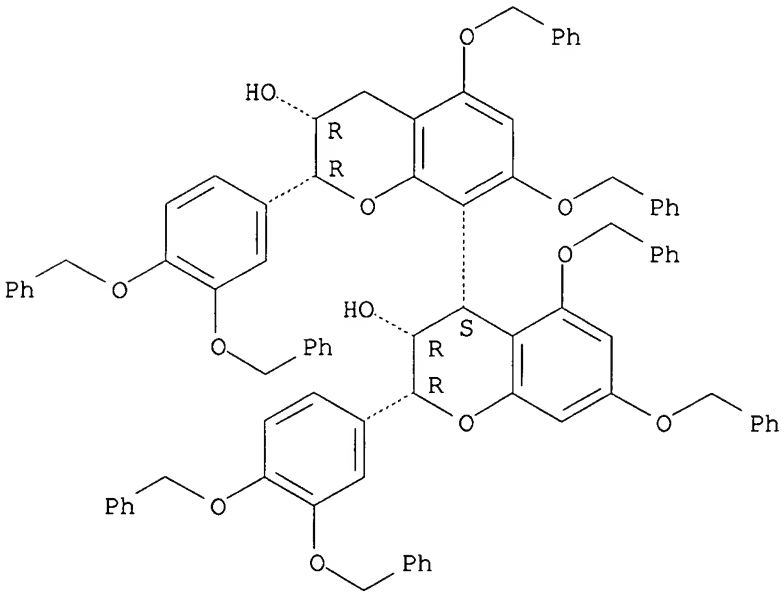


PAGE 2-A



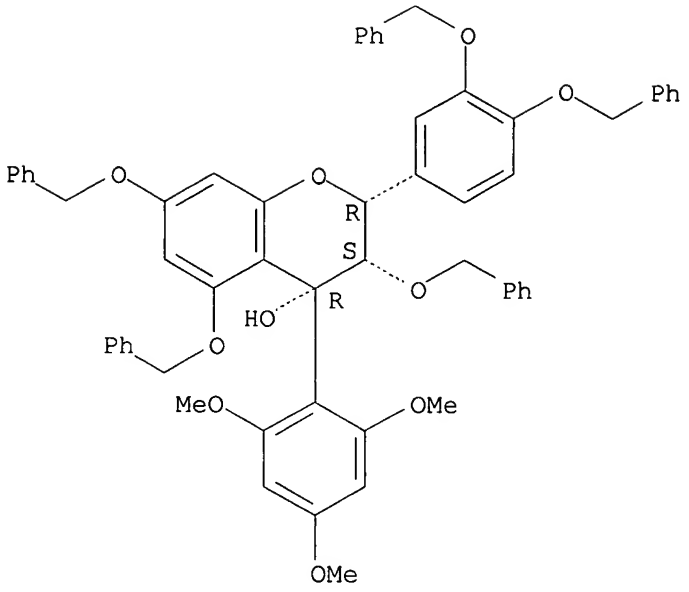
RN 330936-31-7 CAPLUS
CN [4,8'-Bi-2H-1-benzopyran]-3,3'-diol, 2,2'-bis[3,4-bis(phenylmethoxy)phenyl]-3,3',4,4'-tetrahydro-5,5',7,7'-tetrakis(phenylmethoxy)-, (2R,2'R,3R,3'R,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 403651-95-6 CAPLUS
CN 2H-1-Benzopyran-4-ol, 2-[3,4-bis(phenylmethoxy)phenyl]-3,4-dihydro-3,5,7-tris(phenylmethoxy)-4-(2,4,6-trimethoxyphenyl)-, (2R,3S,4R)- (9CI) (CA INDEX NAME)

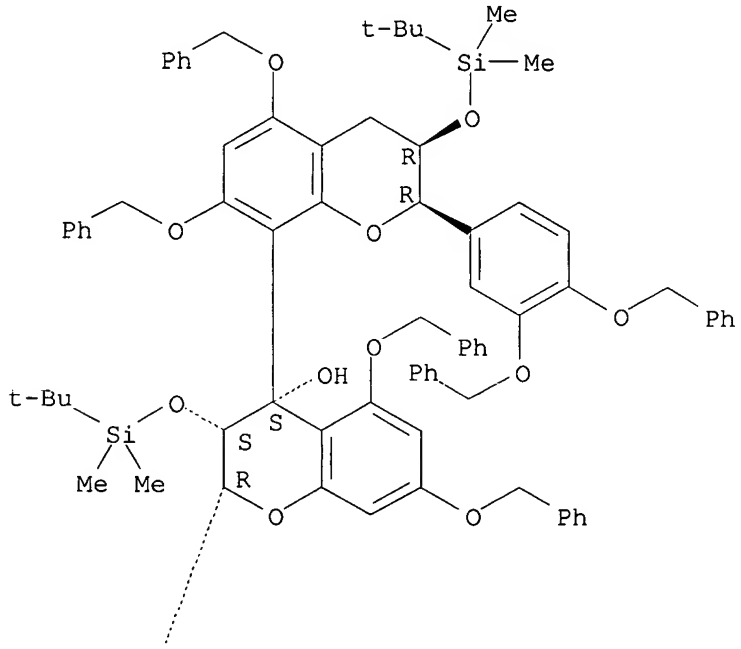
Absolute stereochemistry. Rotation (+).



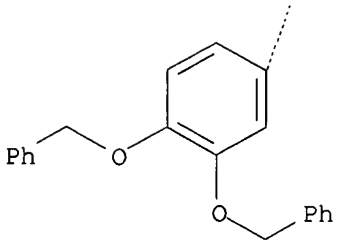
RN 403651-96-7 CAPLUS
CN [4,8'-Bi-2H-1-benzopyran]-4-ol, 2,2'-bis[3,4-bis(phenylmethoxy)phenyl]-3,3'-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-3,3',4,4'-tetrahydro-5,5',7,7'-tetrakis(phenylmethoxy)-, (2R,2'R,3S,3'R,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



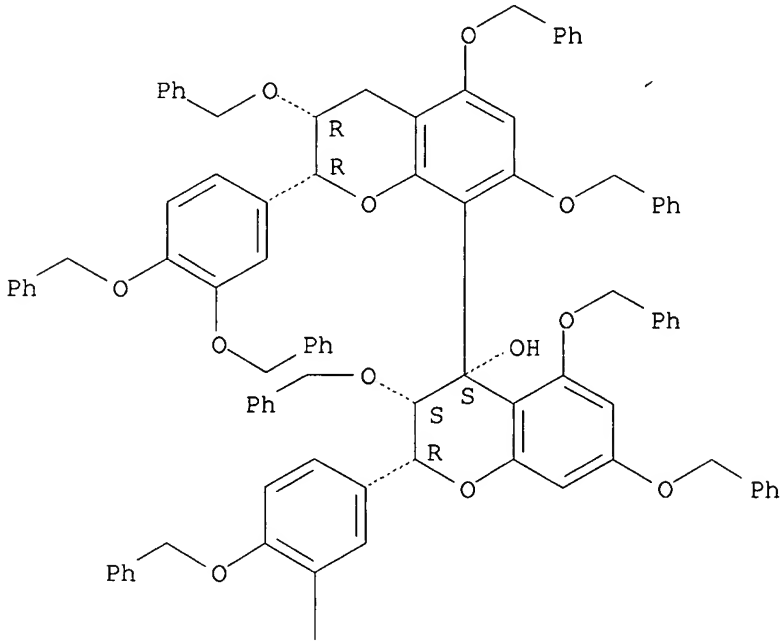
PAGE 2-A



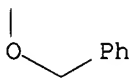
RN 403820-84-8 CAPLUS
CN [4,8'-Bi-4H-1-benzopyran]-4-ol, 2,2'-bis[3,4-bis(phenylmethoxy)phenyl]-2,2',3,3'-tetrahydro-3,3',5,5',7,7'-hexakis(phenylmethoxy)-, (2R,2'R,3S,3'R,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



PAGE 2-A



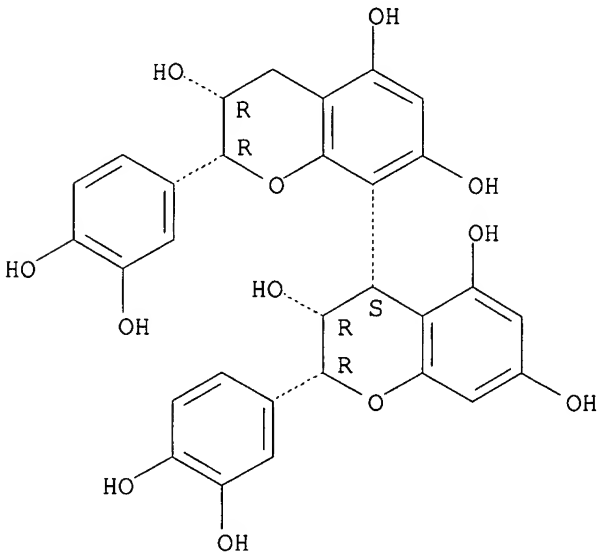
IT **67253-04-7P 67253-05-8P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(**methods** for the **preparation** of 4α-aryl substituted **epicatechin** derivs.)

RN 67253-04-7 CAPLUS

CN [4,8'-Bi-2H-1-benzopyran]-3,3',5,5',7,7'-hexol, 2,2'-bis(3,4-dihydroxyphenyl)-3,3',4,4'-tetrahydro-, (2R,2'R,3R,3'R,4S)- (9CI) (CA INDEX NAME)

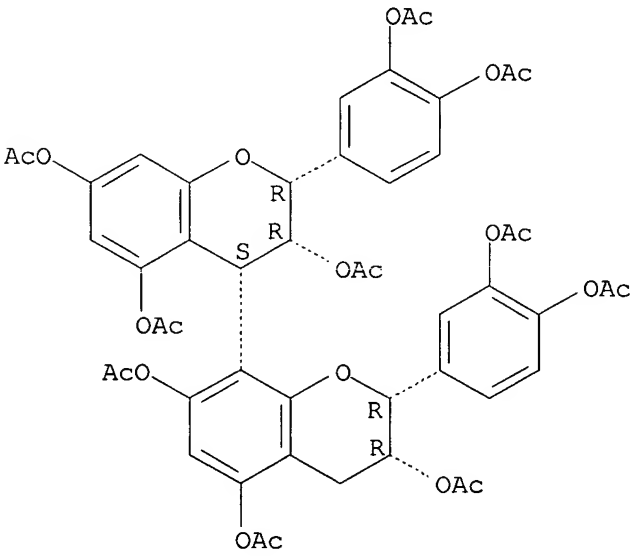
Absolute stereochemistry. Rotation (-).



RN 67253-05-8 CAPLUS

CN [4,8'-Bi-2H-1-benzopyran]-3,3',5,5',7,7'-hexol, 2,2'-bis[3,4-bis(acetyloxy)phenyl]-3,3',4,4'-tetrahydro-, hexaacetate, (2R,2'R,3R,3'R,4S)- (9CI) (CA INDEX NAME)

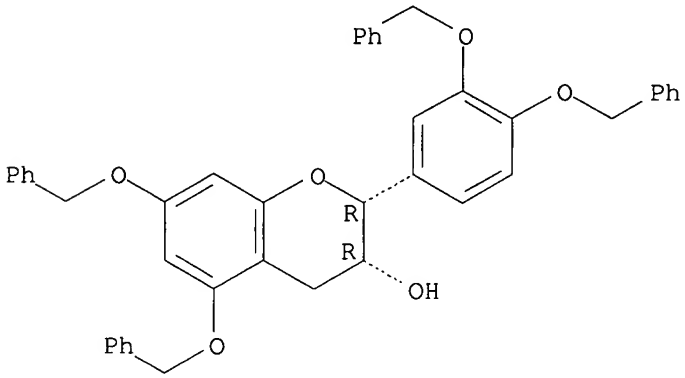
Absolute stereochemistry. Rotation (-).



IT **87292-49-7 223387-36-8 256236-21-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**methods** for the **preparation** of 4α-aryl substituted **epicatechin** derivs.)

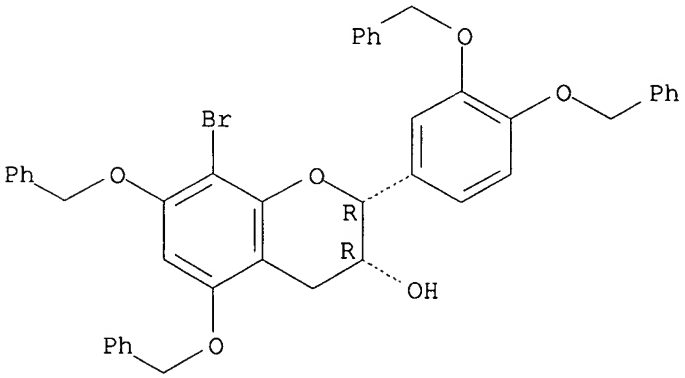
RN 87292-49-7 CAPLUS
CN 2H-1-Benzopyran-3-ol, 2-[3,4-bis(phenylmethoxy)phenyl]-3,4-dihydro-5,7-bis(phenylmethoxy)-, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



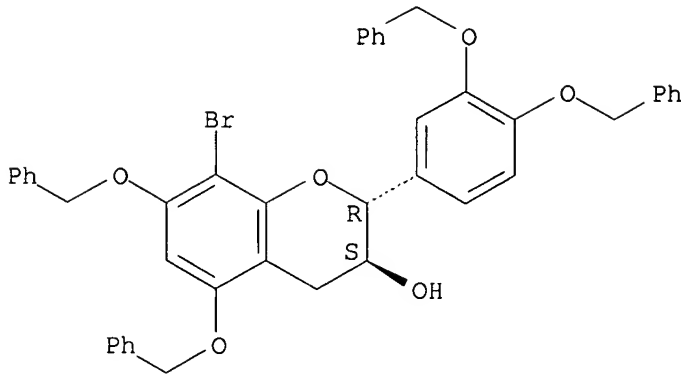
RN 223387-36-8 CAPLUS
CN 2H-1-Benzopyran-3-ol, 2-[3,4-bis(phenylmethoxy)phenyl]-8-bromo-3,4-dihydro-5,7-bis(phenylmethoxy)-, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

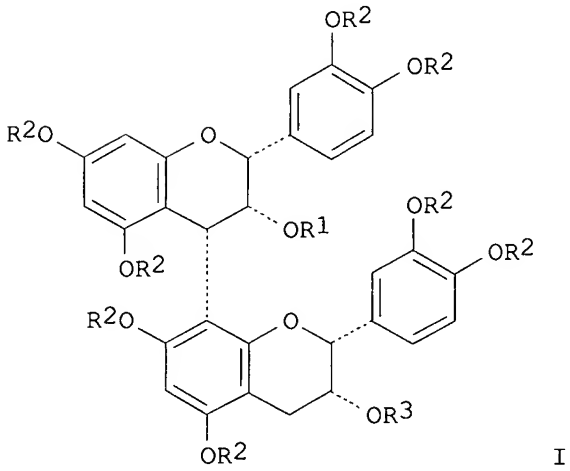


RN 256236-21-2 CAPLUS
CN 2H-1-Benzopyran-3-ol, 2-[3,4-bis(phenylmethoxy)phenyl]-8-bromo-3,4-dihydro-5,7-bis(phenylmethoxy)-, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



GI



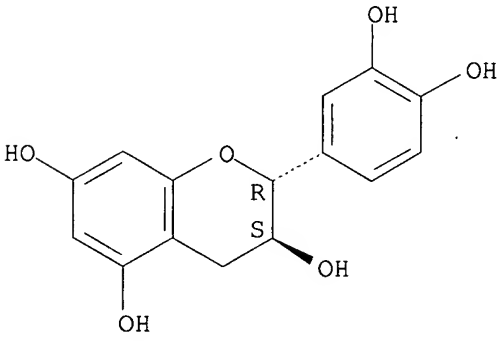
I

AB **Process** for **preparing** a 4α-aryl substituted **epicatechin** derivative including 4α,8- **epicatechin dimers** such as I (R1,R3 = H, acetyl, protected galloyl, galloyl; R2 = H, benzyl, acetyl), is disclosed which comprises the steps of: (a) protecting C-3 hydroxyl group of 5,7,3',4'-tetra-O-benzylepicatechin; (b) **oxidizing** the 4-position of the compound of step (a) to produce protected flavan-4-one; (c) reacting the compound of step (b) with aryllithium reagents, derived by halogen/metal exchange from the aryl bromides, to form C-3 protected 4-hydroxy-4-aryl **epicatechin** derivative; (d) deoxygenating the C-4 position of the compound of step (c) with tri-n-butyltin hydride and trifluoroacetic acid, to afford C-3 protected 4α-aryl-5,7,3',4'-tetra-O-benzylepicatechin. Thus, **epicatechin**-4α,8-(3-O-galloylepicatechin) I (R1, R2 = H; R3 = galloyl) was **prepared** in a multistep synthetic sequence starting from 5,7,3',4'-tetra-O-benzylepicatechin, 5,7,3',4'-tetra-O-benzyl-8-bromoepicatechin, and tri-O-benzyl gallic acid.

L10 ANSWER 9 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:408634 CAPLUS
DOCUMENT NUMBER: 135:45464
TITLE: Changes of (+)-**catechin** antioxidant activity during enzymic **oxidation**
AUTHOR(S): Sosnowska, Dorota
CORPORATE SOURCE: Inst. Biochem. Tech., Politech. Lodzka, Lodz, 90-924, Pol.
SOURCE: Zywnosc (2000), 7(3, Supl.), 69-76
CODEN: ZYWNFL
PUBLISHER: Polskie Towarzystwo Technologow Zywnosci, Oddzial Malopolski
DOCUMENT TYPE: Journal
LANGUAGE: Polish
IT **154-23-4**, +**Catechin**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(antioxidant activity of (+)-**catechin** changes during enzymic **oxidation** with apple polyphenol oxidase and tyrosinase)
RN 154-23-4 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



AB The effects of enzymic **oxidation** of com. pure (+)-**catechin** on its antioxidant activity were investigated. The **oxidation** of (+)-**catechin**, a common component of fruits and vegetables, with apple polyphenol oxidase (PPO) and tyrosinase was studied at 25°C in solns. at pH 4 and 7. The antioxidant activity was determined by 2,2'-azinobis-3(ethylbenzothiazoline-6-sulfonic acid) (ABTS) and 1,1-diphenyl-2-picrylhydrazyl (DPPH) radical scavenging. The (+)-**catechin** and its reaction products were monitored by HPLC and TLC. The rate of **oxidation** reaction in the presence of PPO at pH 7 was higher than at pH 4. The reaction products of **catechin** **oxidation** were **dimers** and tetramers. The **oxidation** of **catechin** with tyrosinase was slower than with PPO. The antioxidant activity of **catechin** after 2 h **oxidation** (PPO at pH 7) was decreased .apprx.25% as determined by the DPPH **method** (expressed as IC50) and .apprx.12% as determined by the ABTS **method** (expressed as TEAC - Trolox Equivalent antioxidant capacity) despite large decrease in the content of monomeric **catechin** (57%). This indicates that (+)-**catechin** enzymic **oxidation** produces compds. with antioxidant activities.

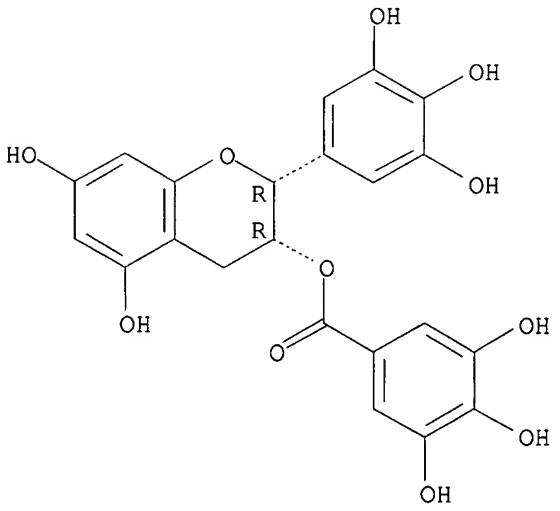
L10 ANSWER 10 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:830787 CAPLUS

DOCUMENT NUMBER: 134:125908
TITLE: Evaluation of the Antioxidant and Pro-oxidant Effects of Tea **Catechin** Oxypolymers
AUTHOR(S): Li, Chunmei; Xie, Bijun
CORPORATE SOURCE: Department of Food Science and Technology, Huazhong Agriculture University, Wuhan, Hubei, 430070, Peop. Rep. China
SOURCE: Journal of Agricultural and Food Chemistry (2000), 48(12), 6362-6366
CODEN: JAFCAU; ISSN: 0021-8561
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **989-51-5D**, Epigallocatechin gallate, oxypolymers
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(antioxidant and pro-oxidant effects of tea **catechin** oxypolymers)

RN 989-51-5 CAPLUS
CN Benzoic acid, 3,4,5-trihydroxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



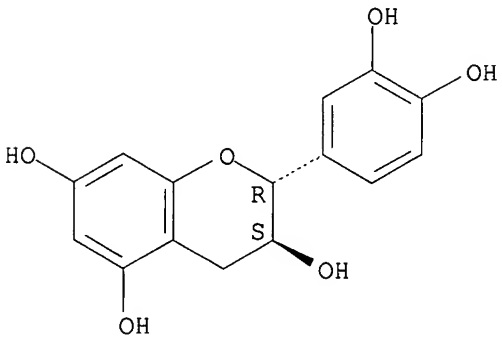
AB Tea **catechin** oxypolymers (TCOP) were **prepared** by **oxidizing** tea **catechin** (TC, the content of epigallocatechin gallate (EGCG) was >85%) with H2O2. TCOP was a mixture of polymers mainly **dimers** and trimers of EGCG. Their antioxidant and pro-oxidant effects were tested using a deoxyribose assay, a photoredn. of NBT assay, a lipoxygenase assay, a POV assay, and animal tests. The scavenging effects of TCOP to both the hydroxyl radical and superoxide radical were stronger than that of TC, and also they had no pro-oxidant effect; the rate constant for reactions of TC and TCOP for hydroxyl radical were 1.0 + 1010 and (1.4-2.8) + 1010 M-1 S-1, resp. TCOP can inhibit lipid peroxidn. and lipoxygenase effectively, and it also can activate red cell SOD and reduce the MDA content in serum of mice very significantly. These results suggested that the antioxidant activity of TCOP was not less than or even more notable than that of TC.

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS

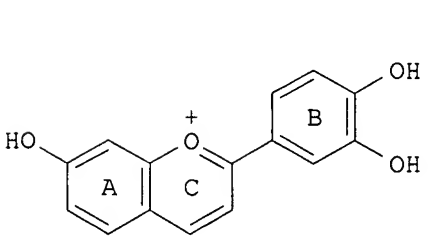
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 11 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:553825 CAPLUS
DOCUMENT NUMBER: 133:335114
TITLE: Antioxidant properties of anthocyanins and tannins: a mechanistic investigation with **catechin** and the 3',4',7-trihydroxyflavylium ion
AUTHOR(S): Dangles, Olivier; Fargeix, Guillaume; Dufour, Claire
CORPORATE SOURCE: UMR-CNRS 5078, Bat. 303, Universite Claude Bernard-Lyon I, Villeurbanne, 69622, Fr.
SOURCE: Perkin 2 (2000), (8), 1653-1663
CODEN: PRKTFO
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:335114
IT **154-23-4, Catechin**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(antioxidant properties of anthocyanins and tannins: a mechanistic investigation with **catechin** and 3',4',7-trihydroxyflavylium ion)
RN 154-23-4 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-, (2R,3S)- (9CI) (CA INDEX NAME)

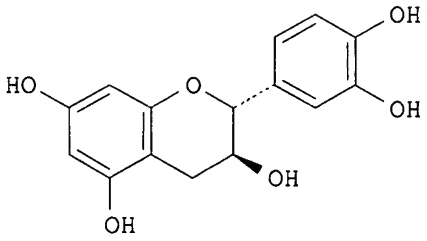
Absolute stereochemistry. Rotation (+).



GI



I



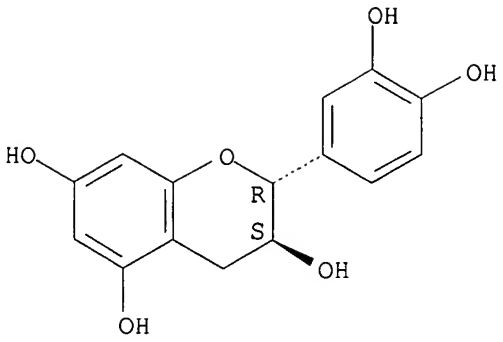
II

AB Plant polyphenols act as antioxidants mainly by trapping reactive oxygen species and by regenerating endogenous membrane-bound α-tocopherol (vitamin E). In both **processes** polyphenols are **oxidized**. Hence, knowledge of the **oxidation** mechanisms of polyphenols is important for an understanding of their antioxidant activity at the mol. level. This work focuses on anthocyanins (pigments) and flavanols (tannins), two important classes of polyphenols which are both relatively abundant in human diet. The **oxidation** of the 3',4',7-trihydroxyflavylium ion (I) and **catechin** (II), resp. taken as models for anthocyanins and tannins, has been investigated. From kinetic data and partial product anal., the mechanisms for the reactions of I and II with sodium periodate and DPPH, a H atom-abstracting radical, are proposed. Both polyphenols are shown to form o-quinone intermediates upon H atom abstraction and subsequent radical disproportionation. In the case of II, the quinone and a second mol. of antioxidant quickly couple to form **dimers**. By contrast, I is extensively degraded into coumarins by repeating sequences of **oxidation**-solvent addition, which consume several equivalent of oxidants. In aqueous solns., I is typically a mixture of colored and colorless forms. The latter (chalcones) are also shown to take part in the antioxidant activity.

REFERENCE COUNT: 73 THERE ARE 73 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

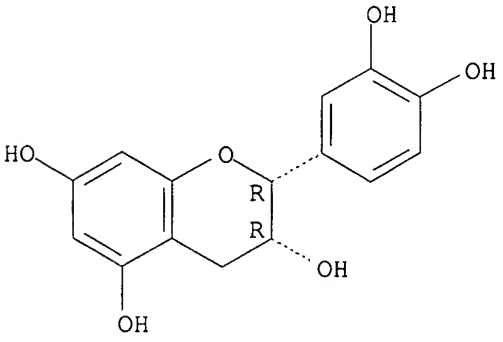
L10 ANSWER 12 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:539327 CAPLUS
DOCUMENT NUMBER: 133:222006
TITLE: **Epicatechin** in human plasma: in vivo determination and effect of chocolate consumption on plasma **oxidation** status
AUTHOR(S): Rein, Dietrich; Lotito, Silvina; Holt, Roberta R.; Keen, Carl L.; Schmitz, Harold H.; Fraga, Cesar G.
CORPORATE SOURCE: Department of Nutrition, University of California, Davis, CA, 95616, USA
SOURCE: Journal of Nutrition (2000), 130(8S), 2109S-2114S
CODEN: JONUAI; ISSN: 0022-3166
PUBLISHER: American Society for Nutritional Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **154-23-4, Catechin**
RL: ANT (Analyte); ANST (Analytical study)
(dietary chocolate effects on **epicatechin** blood plasma kinetics and **oxidation** status in humans)
RN 154-23-4 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT **490-46-0, Epicatechin**
RL: ANT (Analyte); BPR (Biological process); BSU (Biological study, unclassified); FFD (Food or feed use); ANST (Analytical study); BIOL (Biological study); PROC (Process); USES (Uses)
(dietary chocolate effects on **epicatechin** blood plasma kinetics and **oxidation** status in humans)
RN 490-46-0 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



AB Diets rich in plant foods have been associated with decreased risk for specific disease **processes** and certain chronic diseases. In addition to essential macronutrients and micronutrients, flavonoids in plant foods may have health-enhancing properties. Chocolate is rich in the flavan-3-ol **epicatechin** and procyanidin oligomers. The bioavailability and biol. effects of the chocolate flavonoids are poorly understood. HPLC coupled with electrochem. (coulometric) detection was used to determine the physiol. levels of **epicatechin, catechin**, and **epicatechin dimers** in human blood plasma. This **method** allows to determine levels as low as 20 pg (69 fmol) of **epicatechin** (1 nmol/L blood plasma). The absorption of **epicatechin** from an 80-g dose of semisweet procyanidin-rich chocolate was evaluated using this **method** in 13 healthy adult humans. By 2 h after ingestion, there was a 12-fold increase in plasma **epicatechin** levels from 22 to 257 nmol/L. Consistent with the antioxidant properties of **epicatechin**, within the same 2-h period there was a 31% increase in plasma total antioxidant capacity and 40% decrease in the plasma 2-thiobarbituric acid-reactive substance levels. Plasma **epicatechin** and plasma

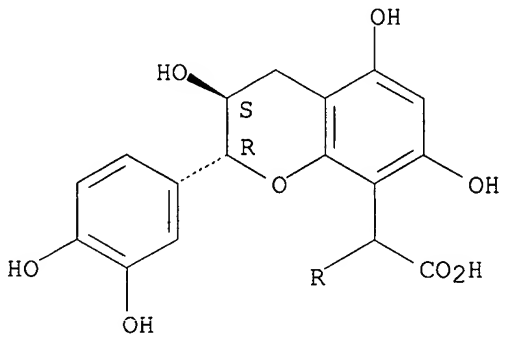
antioxidant capacity approached baseline values by 6 h after chocolate ingestion. Thus, it is possible to determine basal levels of **epicatechin** in blood plasma. The consumption of chocolate can increase blood plasma **epicatechin** and decrease plasma baseline **oxidation** product concns.

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

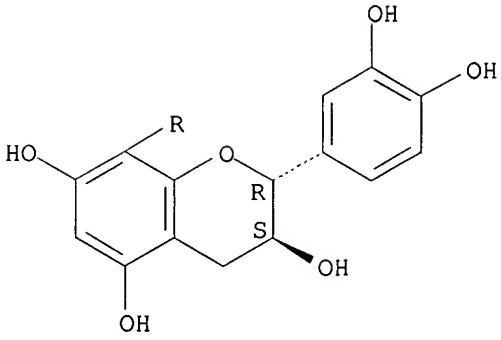
L10 ANSWER 13 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:128621 CAPLUS
DOCUMENT NUMBER: 132:278340
TITLE: Xanthylium salts formation involved in wine color changes
AUTHOR(S): Es-Safi, Nour-Eddine; Le Guerneve, Christine; Fulcrand, Helene; Cheynier, Veronique; Moutounet, Michel
CORPORATE SOURCE: Vigne, Unite de Recherche Biopolymeres et Aromes, ISVV-INRA Institut des Produits, Montpellier, 34060, Fr.
SOURCE: International Journal of Food Science and Technology (2000), 35(1), 63-74
CODEN: IJFTEZ; ISSN: 0950-5423
PUBLISHER: Blackwell Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **246181-58-8**
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
(xanthylium salts formation involved in wine color changes)
RN 246181-58-8 CAPLUS
CN 2H-1-Benzopyran-8-acetic acid, 2-(3,4-dihydroxyphenyl)-α-[(2R,3S)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-3,5,7-trihydroxy-2H-1-benzopyran-8-yl]-3,4-dihydro-3,5,7-trihydroxy-, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

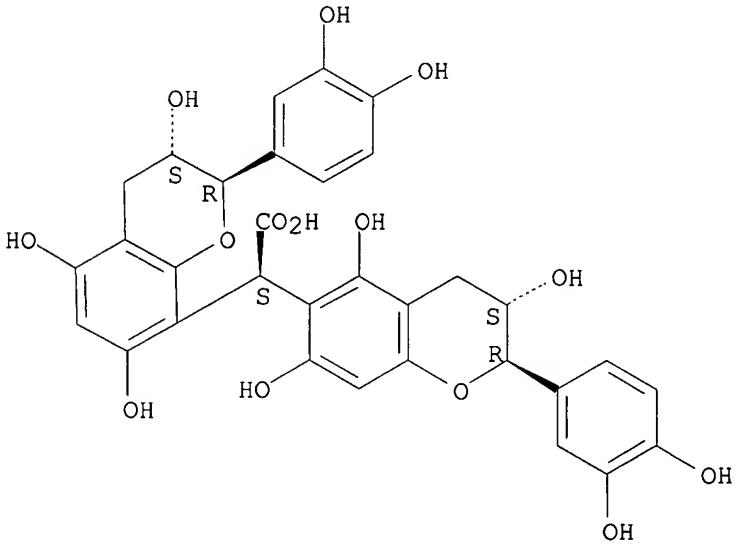


PAGE 2-A



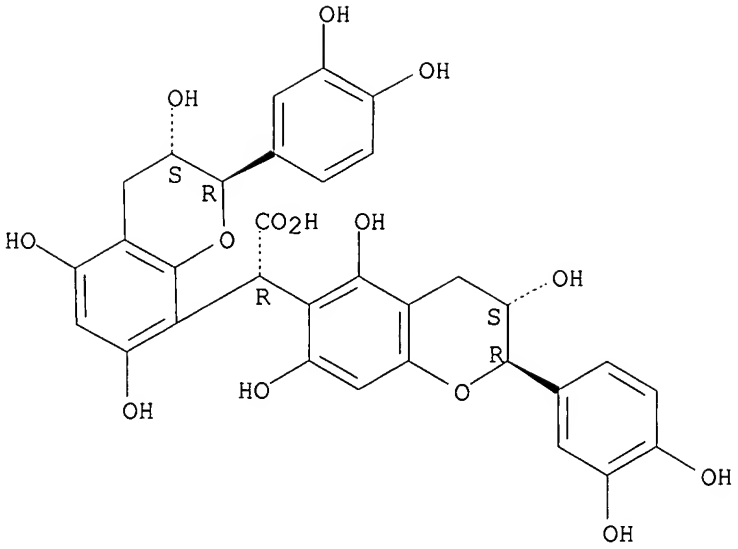
IT **253120-56-8 253120-57-9 253120-58-0**
RL: FMU (Formation, unclassified); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
(xanthylium salts formation involved in wine color changes)
RN 253120-56-8 CAPLUS
CN 2H-1-Benzopyran-6-acetic acid, 2-(3,4-dihydroxyphenyl)-α-[(2R,3S)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-3,5,7-trihydroxy-2H-1-benzopyran-8-yl]-3,4-dihydro-3,5,7-trihydroxy-, (αS,2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



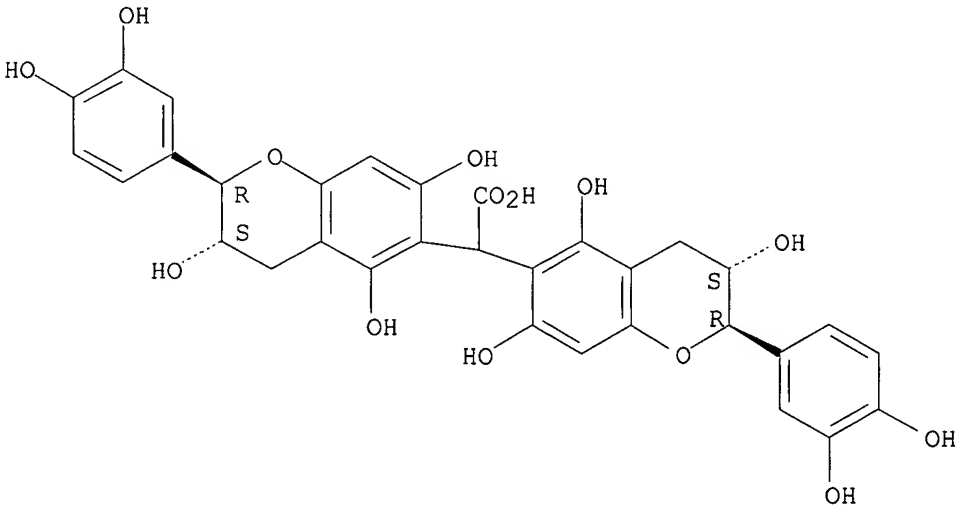
RN 253120-57-9 CAPLUS
CN 2H-1-Benzopyran-6-acetic acid, 2-(3,4-dihydroxyphenyl)-α-[(2R,3S)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-3,5,7-trihydroxy-2H-1-benzopyran-8-yl]-3,4-dihydro-3,5,7-trihydroxy-, (αR,2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



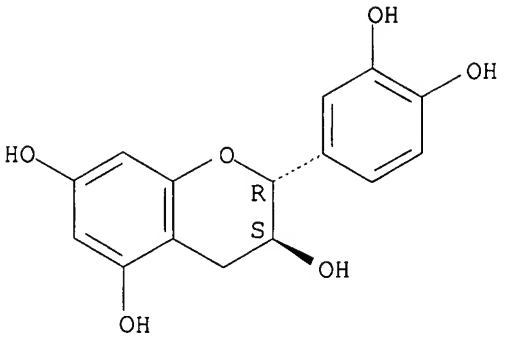
RN 253120-58-0 CAPLUS
CN 2H-1-Benzopyran-6-acetic acid, 2-(3,4-dihydroxyphenyl)-α-[(2R,3S)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-3,5,7-trihydroxy-2H-1-benzopyran-6-yl]-3,4-dihydro-3,5,7-trihydroxy-, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **154-23-4**, (+)-**Catechin**
RL: RCT (Reactant); RACT (Reactant or reagent)
(xanthylium salts formation involved in wine color changes)
RN 154-23-4 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

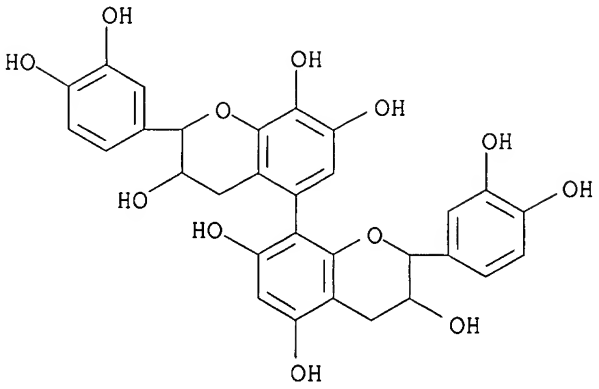


AB The reaction of (+)-**catechin** in wine-like model solution was investigated. First appearance of colorless dimeric compds. consisting of 2 flavanol units linked by carboxymethine bridge was observed Their isolation and further incubation was found to yield 2 types of yellowish pigments showing visible absorption maxima at 440 and 460 nm, resp. Mass spectroscopy (MS) spectral anal. showed that the 1st type were xanthylium salt pigments formed by dehydration of the colorless compds. followed by an **oxidation process**. The loss of a water mol. was shown to take place between 2 A ring hydroxyl groups of the colorless **dimers**. The 2nd type were shown to be ester derivs. of the 1st ones. Thus, the Et ester of xanthylium salt was obtained and fully characterized by mass and NMR spectroscopy. Esterification was found to involve the colorless compound before dehydration and thus a general scheme for xanthylium salt formation was postulated. The proposed scheme constitutes a new xanthylium formation pathway as up to now only anthocyanin-flavanol reactions were supposed to form xanthylium salt derivs. during wine ageing. This work also provides new support to the contribution of xanthylium salt in color evolution observed during wine ageing which is generally expressed in an increase of absorption in the 400-500 nm, region of xanthylium salt absorption maxima.

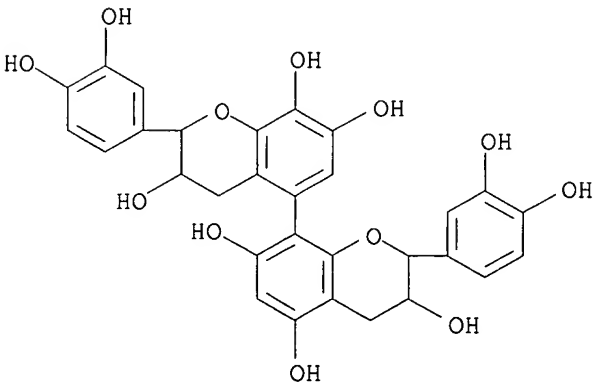
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 14 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:113981 CAPLUS
DOCUMENT NUMBER: 132:251007
TITLE: Tyrosinase catalyzed biphenyl construction from flavan-3-ol substrates
AUTHOR(S): Van Rensburg, Werner Janse; Ferreira, Daneel; Malan, Elfranco; Steenkamp, Jacobus A.
CORPORATE SOURCE: Department of Chemistry, University of the Orange Free State, Bloemfontein, 9300, S. Afr.
SOURCE: Phytochemistry (2000), 53(2), 285-292
CODEN: PYTCAS; ISSN: 0031-9422
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:251007
IT **109671-61-6P 109718-27-6P**
RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(tyrosinase catalyzed biphenyl construction from flavan-3-ol substrates)
RN 109671-61-6 CAPLUS
CN [5,8'-Bi-2H-1-benzopyran]-3,3',5',7,7',8-hexol, 2,2'-bis(3,4-

dihydroxyphenyl)-3,3',4,4'-tetrahydro-, (2R,2'R,3S,3'S,5S)- (9CI) (CA INDEX NAME)

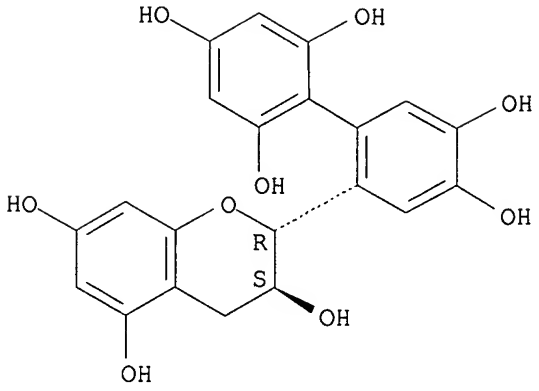


RN 109718-27-6 CAPLUS
CN [5,8'-Bi-2H-1-benzopyran]-3,3',5',7,7',8-hexol, 2,2'-bis(3,4-dihydroxyphenyl)-3,3',4,4'-tetrahydro-, (2R,2'R,3S,3'S,5R)- (9CI) (CA INDEX NAME)



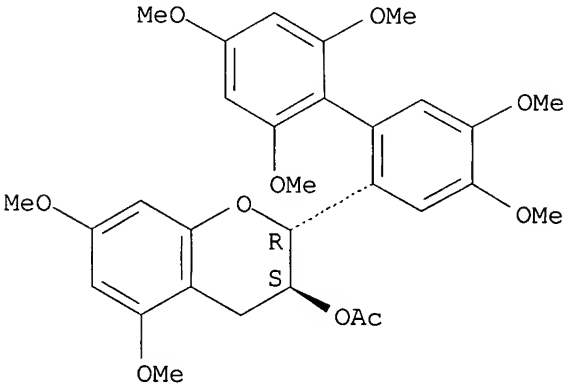
IT **30825-50-4P**
RL: BPN (Biosynthetic preparation); RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(tyrosinase catalyzed biphenyl construction from flavan-3-ol substrates)
RN 30825-50-4 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 3,4-dihydro-2-(2',4,4',5,6'-pentahydroxy[1,1'-biphenyl]-2-yl)-, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



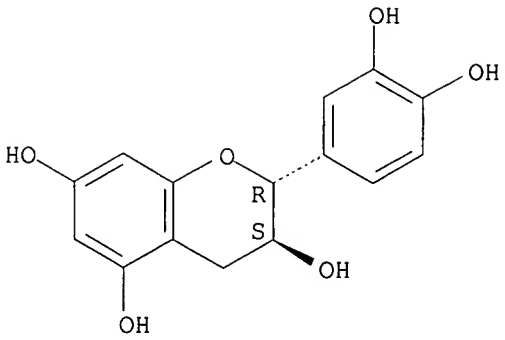
IT **263026-49-9P**
RL: BPN (Biosynthetic preparation); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(tyrosinase catalyzed biphenyl construction from flavan-3-ol substrates)
RN 263026-49-9 CAPLUS
CN 2H-1-Benzopyran-3-ol, 3,4-dihydro-5,7-dimethoxy-2-(2',4,4',5,6'-pentamethoxy[1,1'-biphenyl]-2-yl)-, acetate, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **154-23-4, Catechin**
RL: RCT (Reactant); RACT (Reactant or reagent)
(tyrosinase catalyzed biphenyl construction from flavan-3-ol substrates)
RN 154-23-4 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

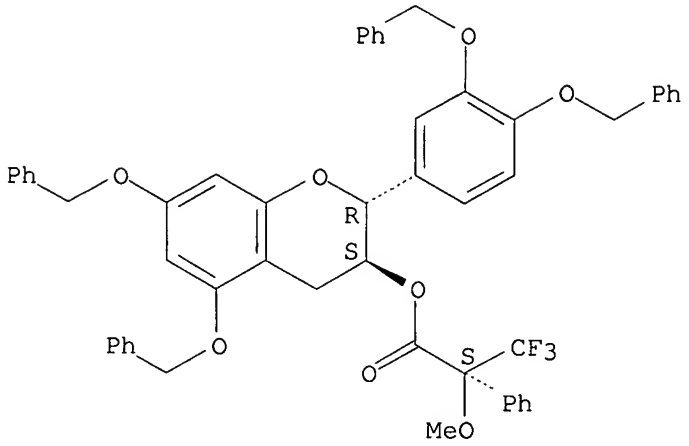


AB Mushroom tyrosinase catalyzed **oxidation** of three flavan-3-ols, viz. **catechin**, fisetinidol and mesquitol, was conducted to construct biphenyl bonds. Exposure of the flavan-3-ols to tyrosinase and subsequent trapping of the o-quinone intermediates resulted in the formation of novel flavan-3-ol derivs., the structures of which were elucidated by mono- and two-dimensional 1H-NMR expts. Application of the methodol. resulted in the improved **synthesis** of the natural flavan-3-ol **dimer**, mesquitol-[5 → 8]- **catechin**, previously isolated from Prosopis glandulosa.

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

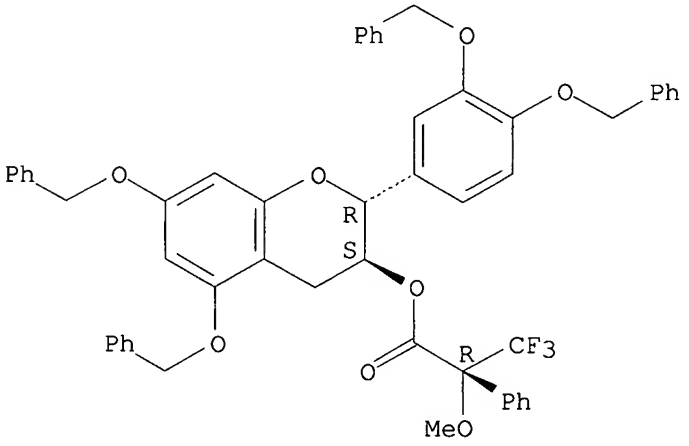
L10 ANSWER 15 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:771159 CAPLUS
DOCUMENT NUMBER: 132:122417
TITLE: Studies in Polyphenol Chemistry and Bioactivity. 1. **Preparation** of Building Blocks from (+)-**Catechin**. Procyanidin Formation. **Synthesis** of the Cancer Cell Growth Inhibitor, 3-O-Galloyl-(2R,3R)-**epicatechin** -4β,8-[3-O-galloyl-(2R,3R)- **epicatechin**]
AUTHOR(S): Tueckmantel, Werner; Kozikowski, Alan P.; Romanczyk, Leo J. ,Jr.
CORPORATE SOURCE: Georgetown University Medical Center Institute for Cognitive and Computational Sciences Drug Discovery Program, Washington, DC, 20007, USA
SOURCE: Journal of the American Chemical Society (1999), 121(51), 12073-12081
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:122417
IT **256236-26-7P 256236-27-8P 256236-28-9P 256236-29-0P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(**synthesis** of [(2R,3R)-3-O-galloylepicatechin]-4β,8-[-(2R,3R)-3-O-galloylepicatechin] from (+)-**catechin**)
RN 256236-26-7 CAPLUS
CN Benzeneacetic acid, α-methoxy-α-(trifluoromethyl)-, (2R,3S)-2-[3,4-bis(phenylmethoxy)phenyl]-3,4-dihydro-5,7-bis(phenylmethoxy)-2H-1-benzopyran-3-yl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



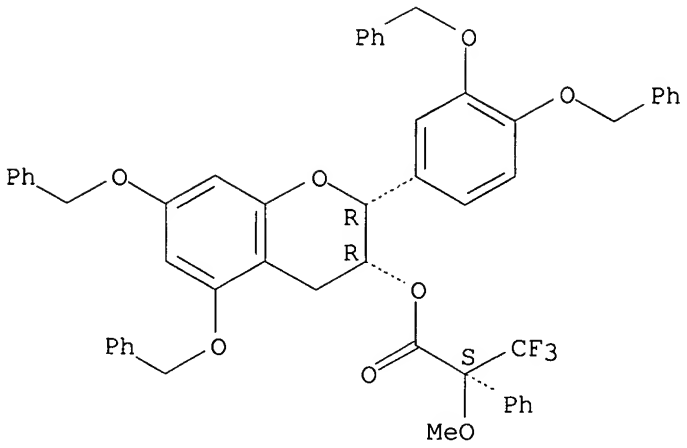
RN 256236-27-8 CAPLUS
CN Benzeneacetic acid, α-methoxy-α-(trifluoromethyl)-, (2R,3S)-2-[3,4-bis(phenylmethoxy)phenyl]-3,4-dihydro-5,7-bis(phenylmethoxy)-2H-1-benzopyran-3-yl ester, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



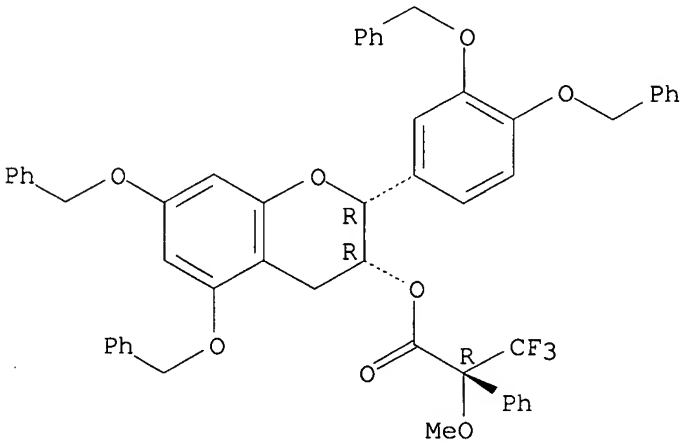
RN 256236-28-9 CAPLUS
CN Benzeneacetic acid, α-methoxy-α-(trifluoromethyl)-, (2R,3R)-2-[3,4-bis(phenylmethoxy)phenyl]-3,4-dihydro-5,7-bis(phenylmethoxy)-2H-1-benzopyran-3-yl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



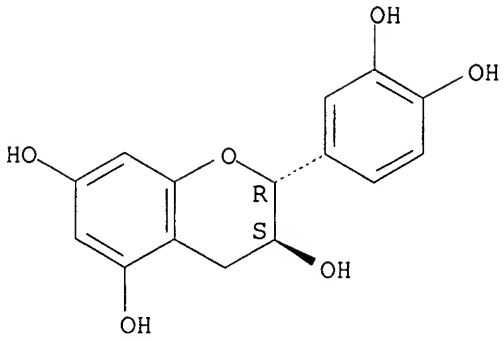
RN 256236-29-0 CAPLUS
CN Benzeneacetic acid, α-methoxy-α-(trifluoromethyl)-, (2R,3R)-2-[3,4-bis(phenylmethoxy)phenyl]-3,4-dihydro-5,7-bis(phenylmethoxy)-2H-1-benzopyran-3-yl ester, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **154-23-4**, (+)-**Catechin**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**synthesis** of [(2R,3R)-3-O-galloylepicatechin]-4β,8-[-(2R,3R)-3-O-galloylepicatechin] from (+)-**catechin**)
RN 154-23-4 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

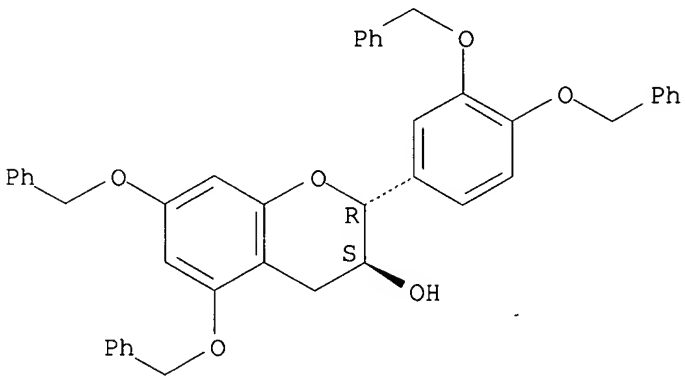


IT **20728-73-8P**, 5,7,3',4'-Tetra-O-benzylcatechin **29106-49-8P**, (+)-Procyanidin B2 **79907-44-1P**, (2R,3R)-3-O-Galloylepicatechin-4β,8-[(2R,3R)-3-O-galloylepicatechin] **87292-49-7P**, (-)-5,7,3',4'-Tetra-O-benzylepicatechin **223387-28-8P** **223387-33-5P** **256236-21-2P**, (-)-5,7,3',4'-Tetra-O-benzyl-8-bromocatechin **256236-25-6P** **256236-30-3P**, (-)-5,7,3',4'-Tetra-O-benzyl-3-O-(3,4,5-tri-O-benzylgalloyl) **epicatechin**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(**synthesis** of [(2R,3R)-3-O-galloylepicatechin]-4β,8-[-(2R,3R)-3-O-galloylepicatechin] from (+)-**catechin**)

RN 20728-73-8 CAPLUS

CN 2H-1-Benzopyran-3-ol, 2-[3,4-bis(phenylmethoxy)phenyl]-3,4-dihydro-5,7-bis(phenylmethoxy)-, (2R,3S)- (9CI) (CA INDEX NAME)

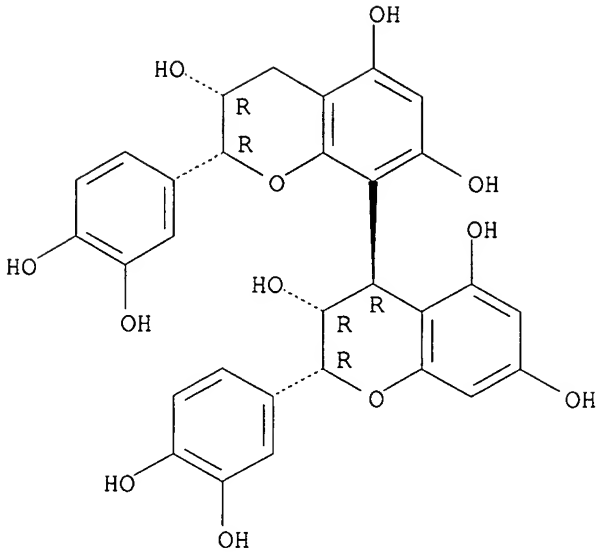
Absolute stereochemistry. Rotation (+).



RN 29106-49-8 CAPLUS

CN [4,8'-Bi-2H-1-benzopyran]-3,3',5,5',7,7'-hexol, 2,2'-bis(3,4-dihydroxyphenyl)-3,3',4,4'-tetrahydro-, (2R,2'R,3R,3'R,4R)- (9CI) (CA INDEX NAME)

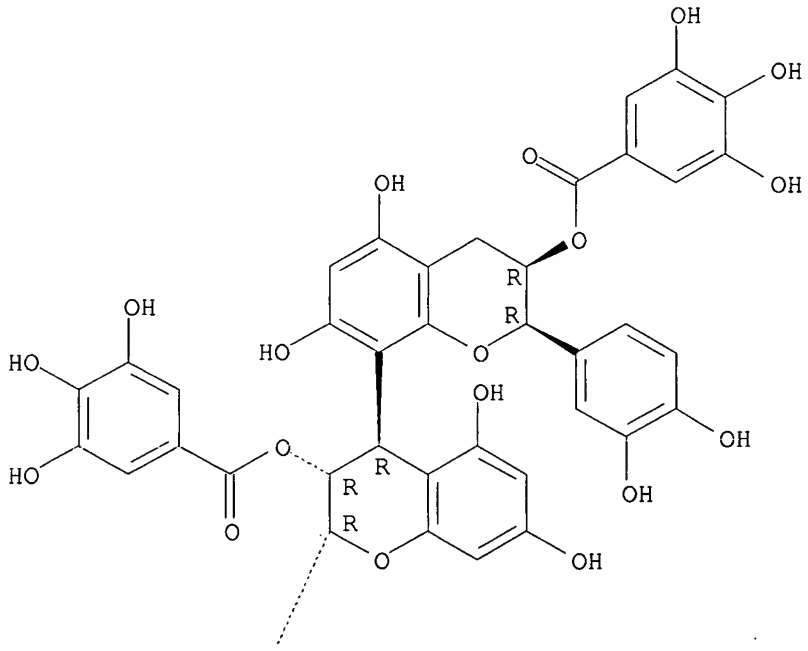
Absolute stereochemistry.

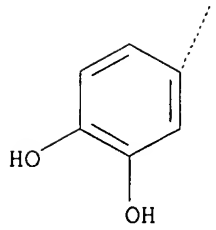


RN 79907-44-1 CAPLUS
CN Benzoic acid, 3,4,5-trihydroxy-, (2R,2'R,3R,3'R,4R)-2,2'-bis(3,4-dihydroxyphenyl)-3,3',4,4'-tetrahydro-5,5',7,7'-tetrahydroxy[4,8'-bi-2H-1-benzopyran]-3,3'-diyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

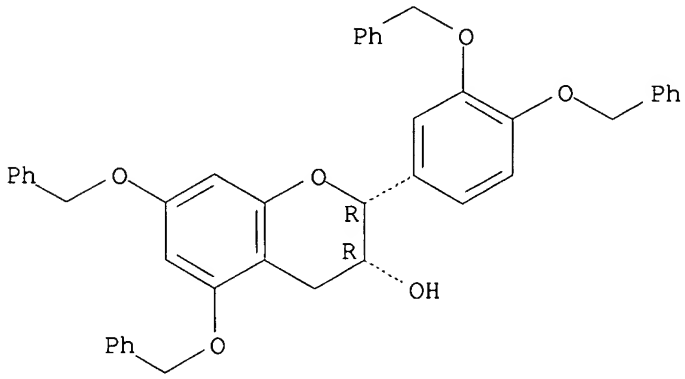
PAGE 1-A





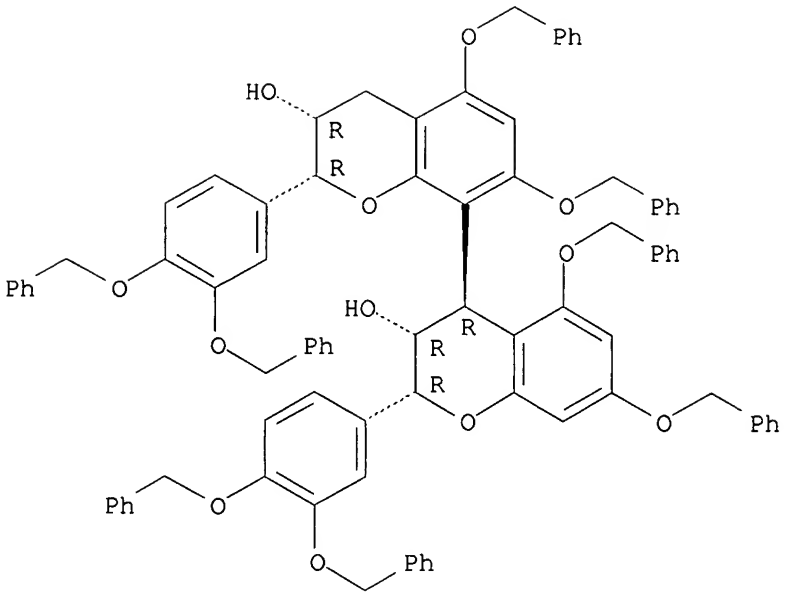
RN 87292-49-7 CAPLUS
CN 2H-1-Benzopyran-3-ol, 2-[3,4-bis(phenylmethoxy)phenyl]-3,4-dihydro-5,7-bis(phenylmethoxy)-, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 223387-28-8 CAPLUS
CN [4,8'-Bi-2H-1-benzopyran]-3,3'-diol, 2,2'-bis[3,4-bis(phenylmethoxy)phenyl]-3,3',4,4'-tetrahydro-5,5',7,7'-tetrakis(phenylmethoxy)-, (2R,2'R,3R,3'R,4R)- (9CI) (CA INDEX NAME)

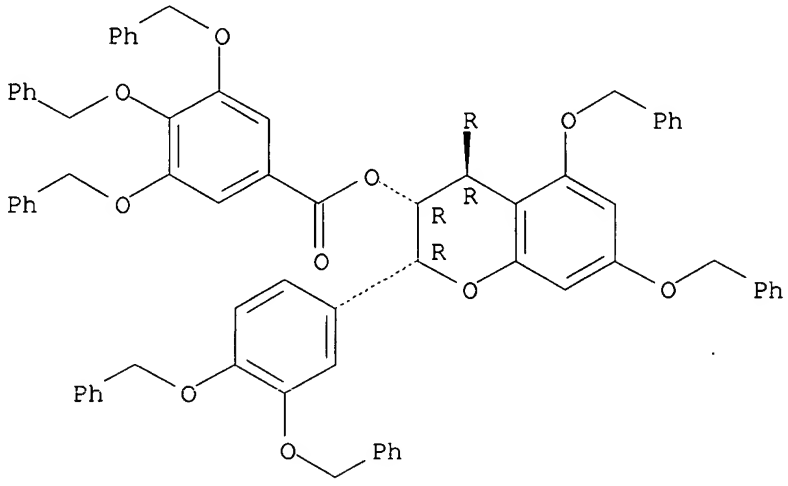
Absolute stereochemistry. Rotation (+).



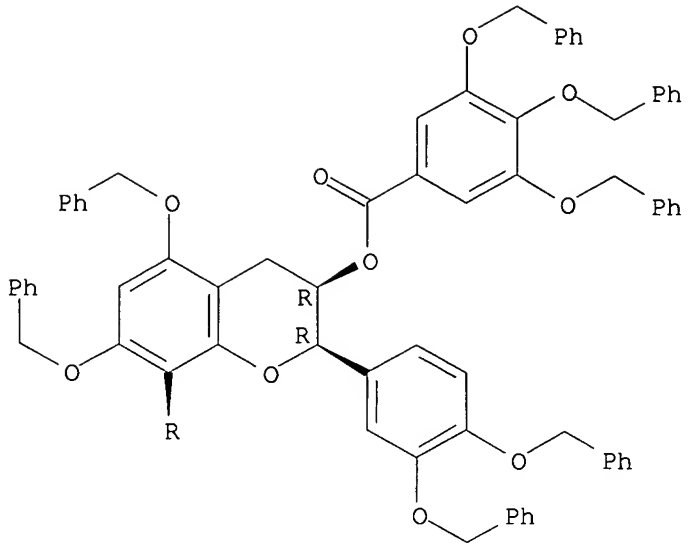
RN 223387-33-5 CAPLUS
CN Benzoic acid, 3,4,5-tris(phenylmethoxy)-, (2R,2'R,3R,3'R,4R)-2,2'-bis[3,4-bis(phenylmethoxy)phenyl]-3,3',4,4'-tetrahydro-5,5',7,7'-tetrakis(phenylmethoxy)[4,8'-bi-2H-1-benzopyran]-3,3'-diyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A

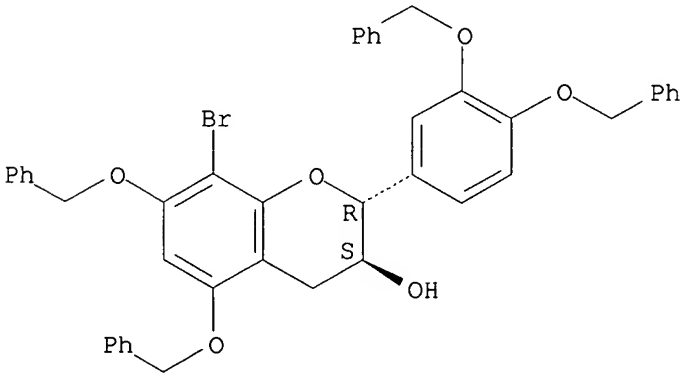


PAGE 2-A



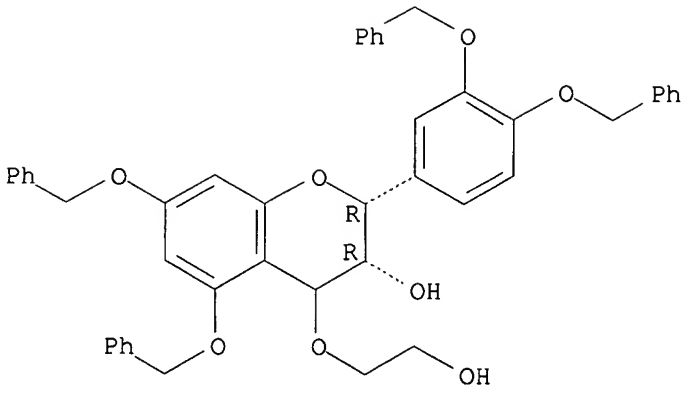
RN 256236-21-2 CAPLUS
CN 2H-1-Benzopyran-3-ol, 2-[3,4-bis(phenylmethoxy)phenyl]-8-bromo-3,4-dihydro-5,7-bis(phenylmethoxy)-, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



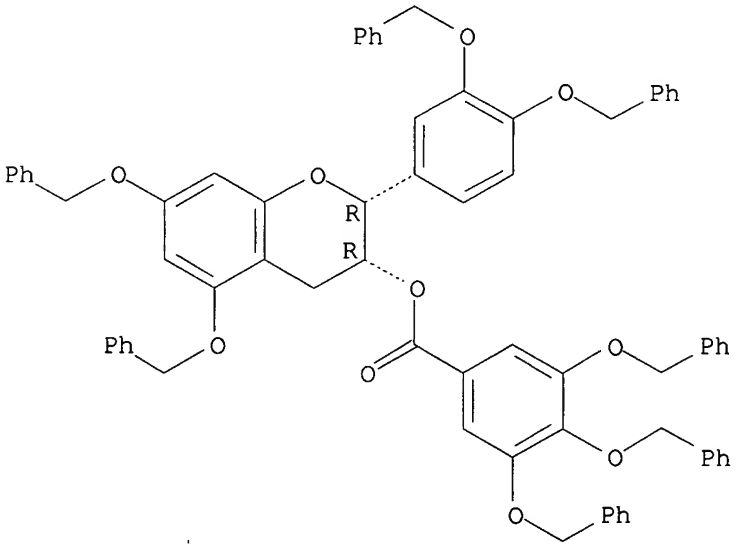
RN 256236-25-6 CAPLUS
CN 2H-1-Benzopyran-3-ol, 2-[3,4-bis(phenylmethoxy)phenyl]-3,4-dihydro-4-(2-hydroxyethoxy)-5,7-bis(phenylmethoxy)-, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



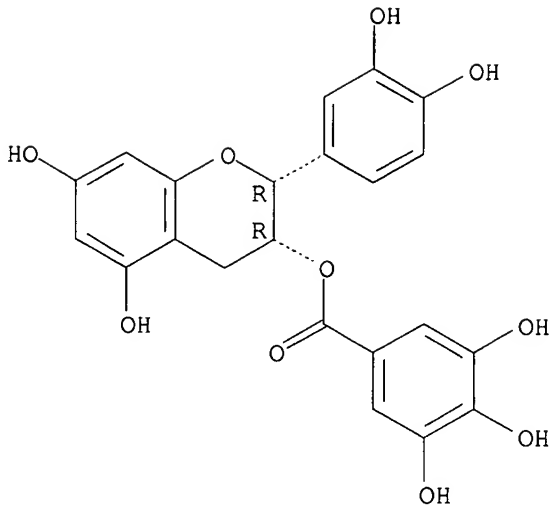
RN 256236-30-3 CAPLUS
CN Benzoic acid, 3,4,5-tris(phenylmethoxy)-, (2R,3R)-2-[3,4-bis(phenylmethoxy)phenyl]-3,4-dihydro-5,7-bis(phenylmethoxy)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



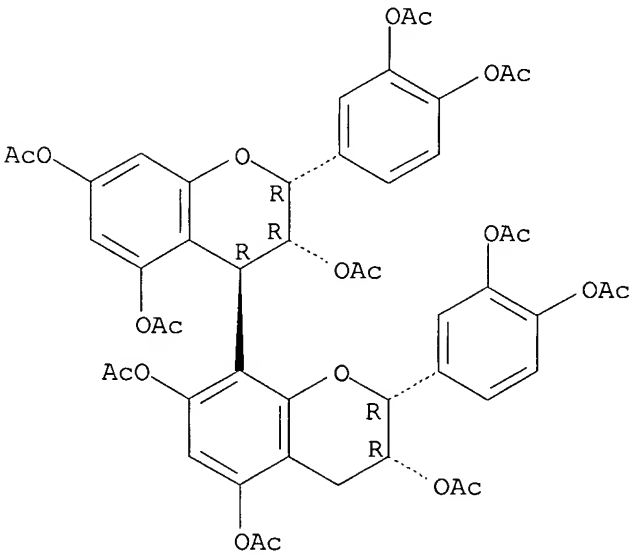
IT **1257-08-5P**, 3-O-Galloylepicatechin **21179-21-5P**, (+)-Procyanidin B2 decaacetate **223387-36-8P**, (-)-8-Bromo-5,7,3',4'-tetra-O-benzylepicatechin **256236-23-4P** **256236-24-5P** **256236-31-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(**synthesis** of [(2R,3R)-3-O-galloylepicatechin]-4β,8-[-(2R,3R)-3-O-galloylepicatechin] from (+)-**catechin**)
RN 1257-08-5 CAPLUS
CN Benzoic acid, 3,4,5-trihydroxy-, (2R,3R)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



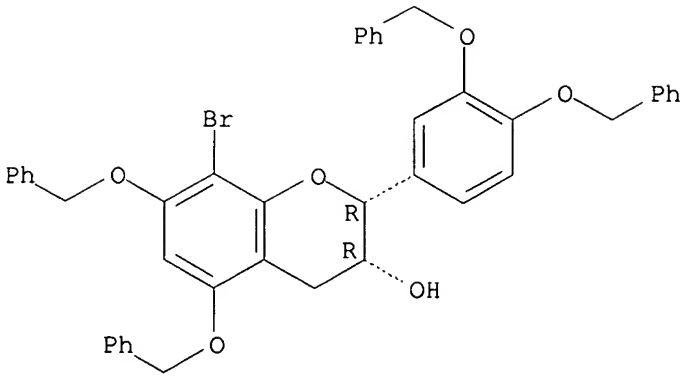
RN 21179-21-5 CAPLUS
CN [4,8'-Bi-2H-1-benzopyran]-3,3',5,5',7,7'-hexol, 2,2'-bis[3,4-bis(acetyloxy)phenyl]-3,3',4,4'-tetrahydro-, hexaacetate, (2R,2'R,3R,3'R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



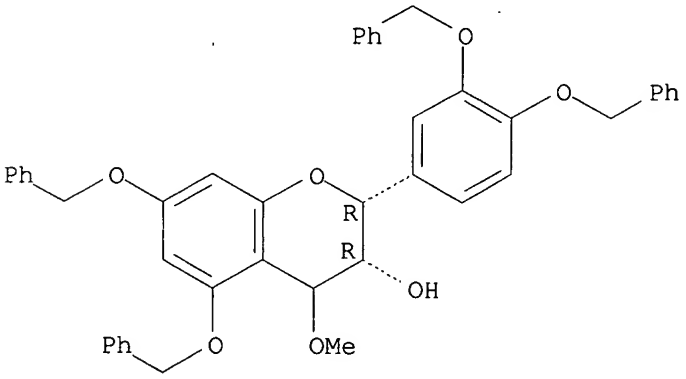
RN 223387-36-8 CAPLUS
CN 2H-1-Benzopyran-3-ol, 2-[3,4-bis(phenylmethoxy)phenyl]-8-bromo-3,4-dihydro-5,7-bis(phenylmethoxy)-, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



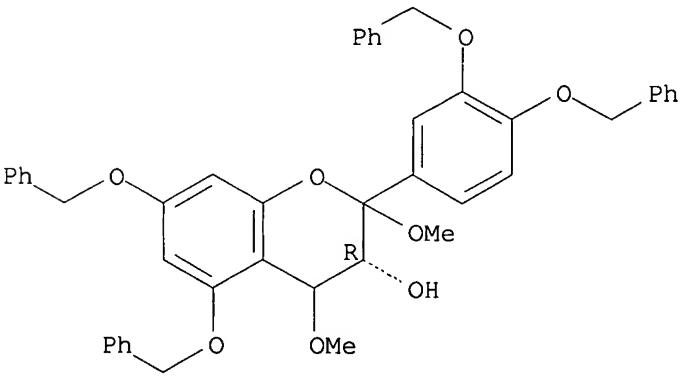
RN 256236-23-4 CAPLUS
CN 2H-1-Benzopyran-3-ol, 2-[3,4-bis(phenylmethoxy)phenyl]-3,4-dihydro-4-methoxy-5,7-bis(phenylmethoxy)-, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



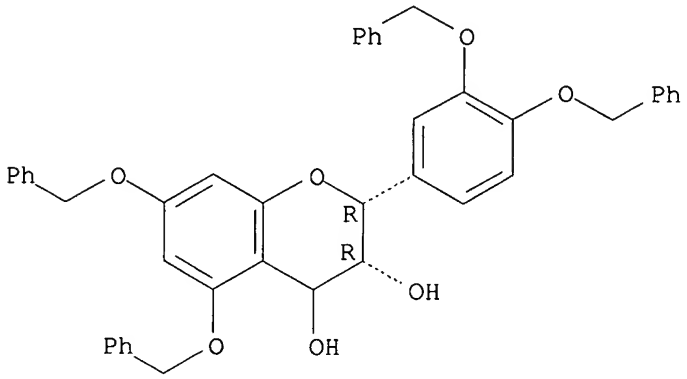
RN 256236-24-5 CAPLUS
CN 2H-1-Benzopyran-3-ol, 2-[3,4-bis(phenylmethoxy)phenyl]-3,4-dihydro-2,4-dimethoxy-5,7-bis(phenylmethoxy)-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 256236-31-4 CAPLUS
CN 2H-1-Benzopyran-3,4-diol, 2-[3,4-bis(phenylmethoxy)phenyl]-3,4-dihydro-5,7-bis(phenylmethoxy)-, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

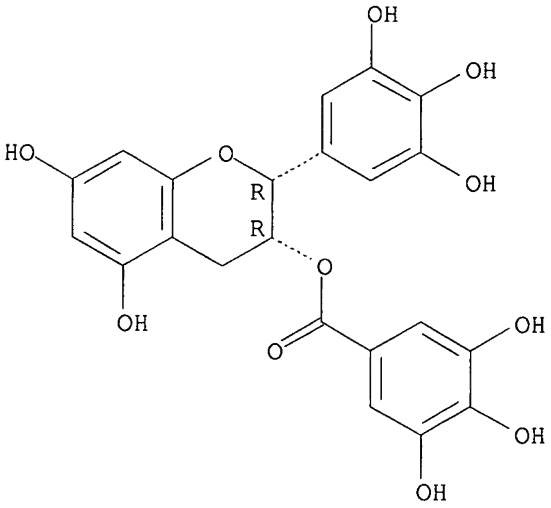
AB A project has been initiated to **synthesize** proanthocyanidin oligomers found in cocoa. Natural, readily available (+)-**catechin** was transformed into 5,7,3',4'-tetra-O-benzyl-(-)-**epicatechin** (I) by (a) benzylation of the phenolic oxygens; (b) **oxidation** of the 3-alc. to ketone by the Dess-Martin periodinane; and (c) reduction with lithium tri-sec-butylborohydride (L-Selectride) in the presence of LiBr. The additive diminishes the extent of ketone enolization while maintaining a stereoselectivity of ≥200:1. **Oxidation** of I with DDQ was performed best from the standpoint of product purification if ethylene glycol was used as the nucleophilic trapping agent. The resulting ether II was condensed with I using TiCl4 to give a good yield of benzyl-protected **epicatechin**-4β,8- **epicatechin** (octa-O-benzylprocyanidin B2, III) as the sole dimeric product. Hydrogenolysis of III yielded procyanidin B2 in the first enantiospecific **synthesis** of this natural product which employs protected intermediates and thereby allows the necessary product separation after the condensation step to be performed on nonpolar, nonsensitive intermediates. Acylation of III with tri-O-benzylgalloyl chloride followed by hydrogenolysis gave access to the title bis-gallate IV [R = COC6H2(OH)3-3,4,5]. This constitutes the first **synthesis** of this natural product, a compound notable for its PKC-inhibitory and anticancer activity.

REFERENCE COUNT: 201 THERE ARE 201 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 16 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:195757 CAPLUS
DOCUMENT NUMBER: 131:5123
TITLE: Antioxidant Chemistry of Green Tea **Catechins**. Identification of Products of the Reaction of

(-)-Epigallocatechin Gallate with Peroxyl Radicals
AUTHOR(S): Valcic, Susanne; Muders, Annette; Jacobsen, Neil E.; Liebler, Daniel C.; Timmermann, Barbara N.
CORPORATE SOURCE: Department of Pharmacology Toxicology College of Pharmacy, The University of Arizona, Tucson, AZ, 85721, USA
SOURCE: Chemical Research in Toxicology (1999), 12(4), 382-386
CODEN: CRTOEC; ISSN: 0893-228X
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **989-51-5**, (-)-Epigallocatechin gallate
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(antioxidant chemical of (-)-epigallocatechin gallate from green tea)
RN 989-51-5 CAPLUS
CN Benzoic acid, 3,4,5-trihydroxy-, (2R,3R)-3,4-dihydro-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-2H-1-benzopyran-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

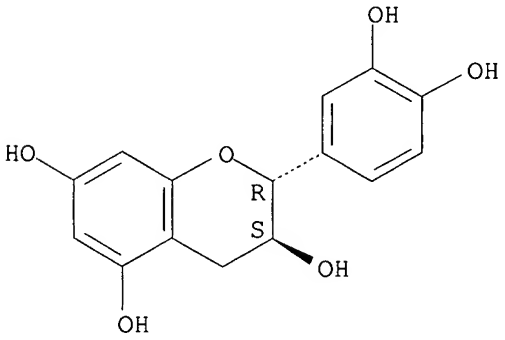


AB (-)-Epigallocatechin gallate (EGCG), isolated from green tea, displays antioxidant properties and is thought to act as an antioxidant in biol. systems. However, the specific mechanisms of its antioxidant actions remain unclear. The authors have isolated and identified for the first time two reaction products of EGCG derived from its reaction with peroxyl radicals generated by thermolysis of the initiator 2,2'-azobis(2,4-dimethylvaleronitrile) (AMVN). The products include a seven-membered B-ring anhydride and a novel **dimer**. The identification of these products provides the first unambiguous proof that the principal site of antioxidant reactions on the EGCG mol. is the trihydroxyphenyl B ring, rather than the 3-galloyl moiety. In contrast to phenoxyl radicals from simple phenolic antioxidants, an initially formed EGCG phenoxyl radical apparently does not form stable addition products with AMVN-derived peroxyl radicals. Characteristic reaction products may provide novel markers for EGCG antioxidant reactions in living systems.
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 17 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:157268 CAPLUS

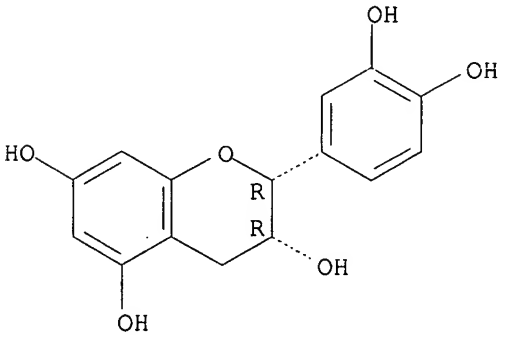
DOCUMENT NUMBER: 130:301542
TITLE: Biochemical activities of extracts from Hypericum perforatum. 3rd communication. Modulation of peroxidase activity as a simple **method** for standardization
AUTHOR(S): Schempp, Harald; Denke, Andrea; Mann, Elke; Schneider, Werner; Elstner, Erich F.
CORPORATE SOURCE: Labor Angewandte Biochemie, Technische Universitaet Muenchen, Freising, D-85350, Germany
SOURCE: Arzneimittel-Forschung (1999), 49(2), 115-119
CODEN: ARZNAD; ISSN: 0004-4172
PUBLISHER: Editio Cantor Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **154-23-4 490-46-0, Epicatechin**
RL: ANT (Analyte); BOC (Biological occurrence); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); OCCU (Occurrence)
(components of Hypericum exts. by HPLC separation)
RN 154-23-4 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 490-46-0 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



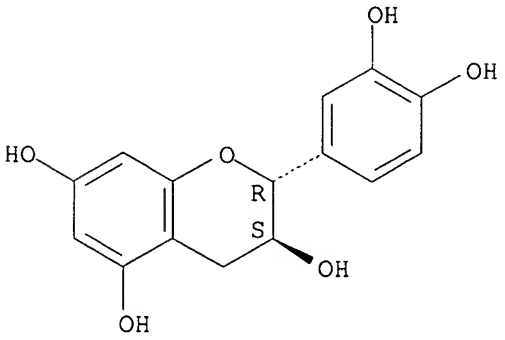
AB Alc. exts. from the herb "St. John's wort" (Hypericum perforatum) are

widely used to counteract depressive situations, where the question on the mainly active principle is still under discussion. Thus, standardization of the drug on the basis of dry matter was chosen instead of the popular leading component, hypericin. Inhibition of myeloperoxidase-catalyzed dimerization of enkephalins by Hypericum exts. was recently reported. This **method** is based on the separation and quantification of enkephalin **dimers** by HPLC. To simplify this assay myeloperoxidase could be substituted by the cheaper horseradish peroxidase and the enkephalins by the amino acid tyrosine without loss of significance. In this communication we represent a more rapid photometric **method** based on peroxidase-catalyzed indole acetic acid **oxidation** suitable for quick, simple, and economic drug standardization.

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 18 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:591261 CAPLUS
DOCUMENT NUMBER: 129:188607
TITLE: Effect of malvidin-3-monoglucoside on the browning of monomeric and dimeric flavanols
AUTHOR(S): Francia-Aricha, E. M.; Rivas-Gonzalo, J. C.; Santos-Buelga, C.
CORPORATE SOURCE: Dep. Quimica Analitica, Nutricion, Bromatologia, Fac. Farmacia, Univ. Salamanca, Salamanca, E-37007, Spain
SOURCE: Zeitschrift fuer Lebensmittel-Untersuchung und -Forschung A: Food Research and Technology (1998), 207(3), 223-228
CODEN: ZLFAFA; ISSN: 1431-4630
PUBLISHER: Springer-Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **154-23-4**, (+)-**Catechin** **490-46-0**, (-)-**Epicatechin** **7228-78-6**, Malvidin-3-monoglucoside **23567-23-9**, Procyanidin B3 **29106-49-8**, Procyanidin B2
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(effect of malvidin-3-monoglucoside on browning of monomeric and dimeric flavanols)
RN 154-23-4 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-, (2R,3S)- (9CI) (CA INDEX NAME)

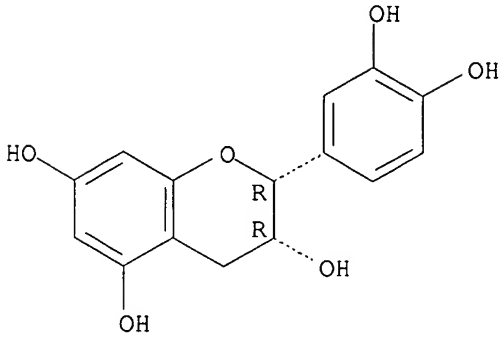
Absolute stereochemistry. Rotation (+).



RN 490-46-0 CAPLUS

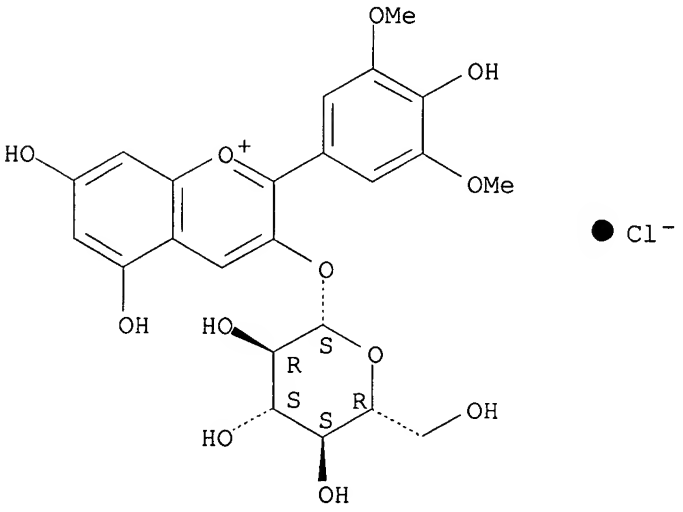
CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



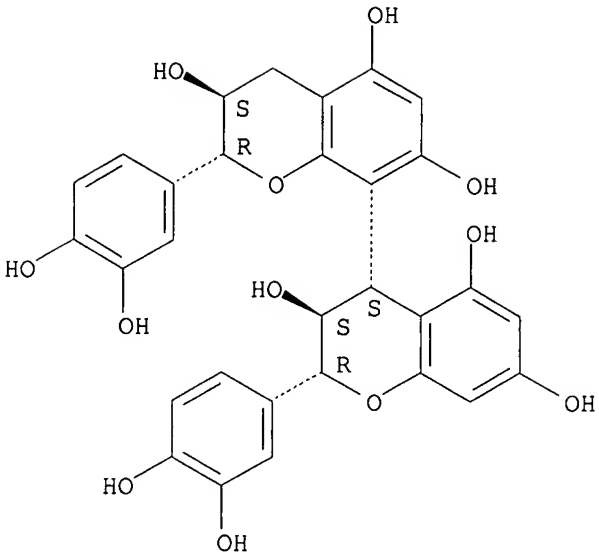
RN 7228-78-6 CAPLUS
CN 1-Benzopyrylium, 3-(β-D-glucopyranosyloxy)-5,7-dihydroxy-2-(4-hydroxy-3,5-dimethoxyphenyl)-, chloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



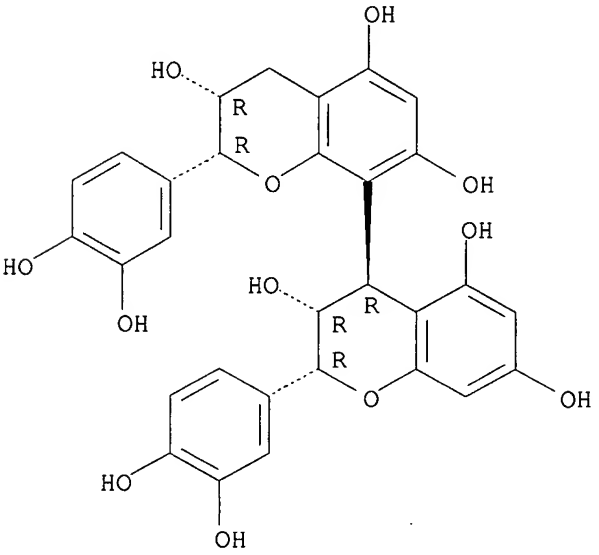
RN 23567-23-9 CAPLUS
CN [4,8'-Bi-2H-1-benzopyran]-3,3',5,5',7,7'-hexol, 2,2'-bis(3,4-dihydroxyphenyl)-3,3',4,4'-tetrahydro-, (2R,2'R,3S,3'S,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 29106-49-8 CAPLUS
CN [4,8'-Bi-2H-1-benzopyran]-3,3',5,5',7,7'-hexol, 2,2'-bis(3,4-dihydroxyphenyl)-3,3',4,4'-tetrahydro-, (2R,2'R,3R,3'R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

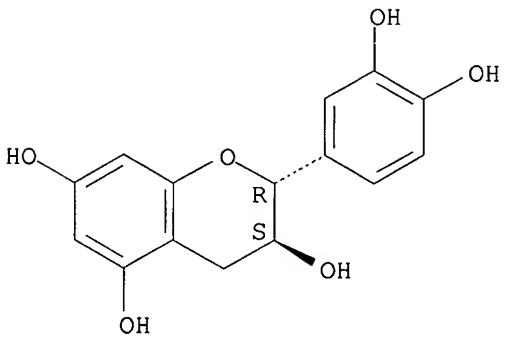


AB The behavior of (+)-**catechin** (cat), (-)-**epicatechin** (epi) and the procyanidin **dimers** B2 [epi-(4 → 8)-epi] and B3 [cat-(4 → 8)-cat], alone and in the presence of malvidin-3-monoglucoside, was studied in hydro-alc. solns. at pH 3.2 maintained at 32° for 120 days. Browning was observed both in the presence and absence of the anthocyanin, except in the solution containing only cat. The formation of pigments showing maximum absorption in the visible region of 440-460 nm was detected. The majority of these new pigments did

not require the anthocyanin for their formation, but rather were derived directly from the flavanol. Some specific pigments showing similar spectra appeared in each of the solns. containing both a flavanol and the anthocyanin, and their production was attributed to a condensation **process** between the two latter compds. The cat units showed a greater tendency to condense with the anthocyanin, while the epi units were more sensitive to chemical **oxidation** The formation of pigments which showed maximum absorbance in the visible region .apprx.530-545 nm, resulting from the condensation between the flavanol and the anthocyanin mediated by acetaldehyde, was also detected. As no acetaldehyde was added to the solns., its presence was attributed to the **oxidation** of ethanol coupled to autoxidn. of the catechol rings of the flavanols.

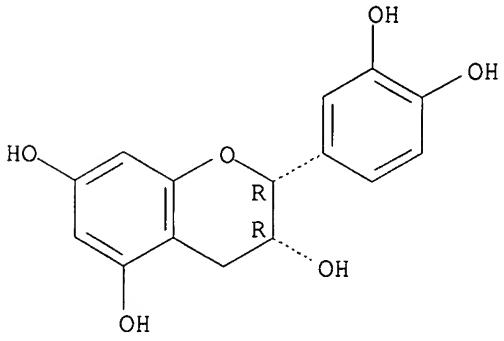
L10 ANSWER 19 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:66516 CAPLUS
DOCUMENT NUMBER: 128:139871
TITLE: Incidence of Molecular Structure in **Oxidation** of Grape Seeds Procyanidins
AUTHOR(S): de Freitas, Victor A. P.; Glories, Yves; Laguerre, Michel
CORPORATE SOURCE: Departamento de Quimica, Faculdade de Ciencias da Universidade do Porto, Oporto, 4150, Port.
SOURCE: Journal of Agricultural and Food Chemistry (1998), 46(2), 376-382
CODEN: JAFCAU; ISSN: 0021-8561
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **154-23-4**, (+)-**Catechin 490-46-0**, (-)-**Epicatechin 12798-58-2**, Procyanidin B6 **12798-59-3**, Procyanidin B7 **12798-60-6**, Procyanidin B8 **20315-25-7**, Procyanidin B1 **23567-23-9**, Procyanidin B3 **29106-49-8**, Procyanidin B2 **29106-51-2**, Procyanidin B4 **37064-30-5**, Procyanidin C1 **73086-04-1 89064-33-5 97233-64-2 201412-28-4 202473-91-4**
RL: BPR (Biological process); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); BIOL (Biological study); PROC (Process)
(incidence of mol. structure in **oxidation** of grape seeds procyanidins)
RN 154-23-4 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



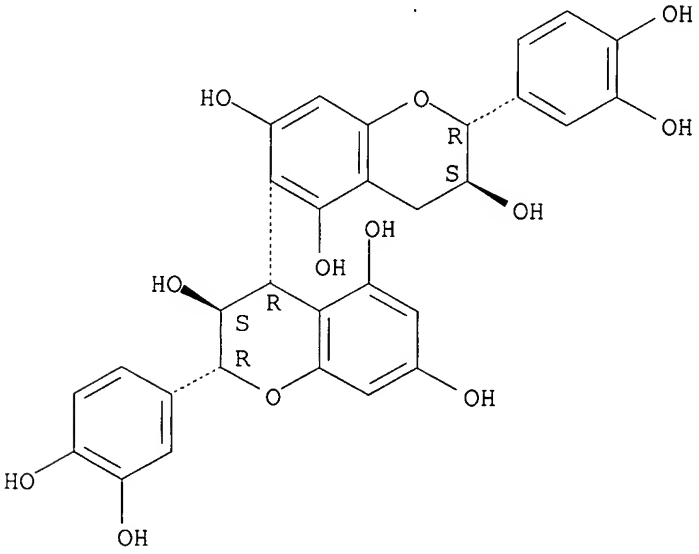
RN 490-46-0 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



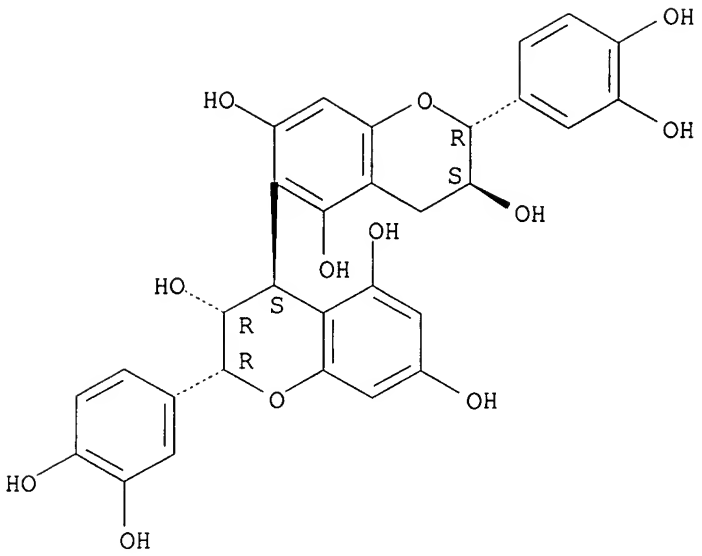
RN 12798-58-2 CAPLUS
CN [4,6'-Bi-2H-1-benzopyran]-3,3',5,5',7,7'-hexol, 2,2'-bis(3,4-dihydroxyphenyl)-3,3',4,4'-tetrahydro-, (2R,2'R,3S,3'S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



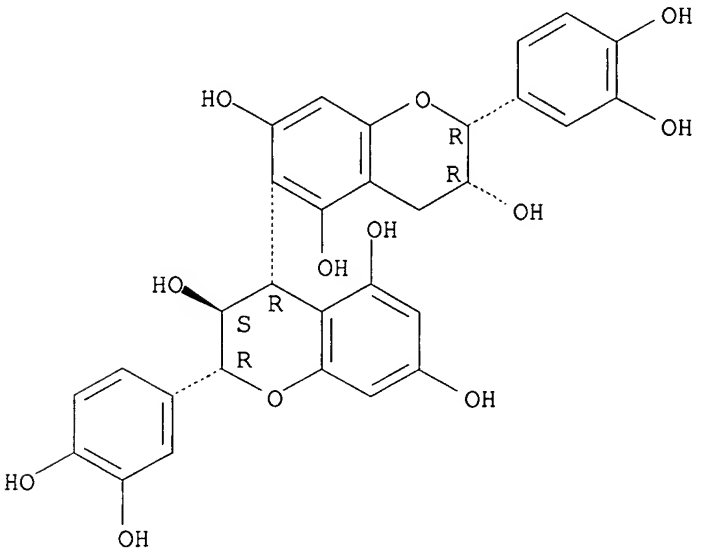
RN 12798-59-3 CAPLUS
CN [4,6'-Bi-2H-1-benzopyran]-3,3',5,5',7,7'-hexol, 2,2'-bis(3,4-dihydroxyphenyl)-3,3',4,4'-tetrahydro-, (2R,2'R,3R,3'S,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



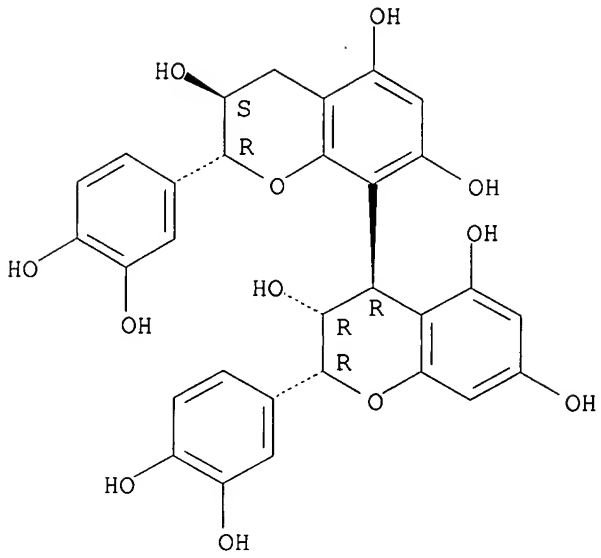
RN 12798-60-6 CAPLUS
CN [4,6'-Bi-2H-1-benzopyran]-3,3',5,5',7,7'-hexol, 2,2'-bis(3,4-dihydroxyphenyl)-3,3',4,4'-tetrahydro-, (2R,2'R,3S,3'R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



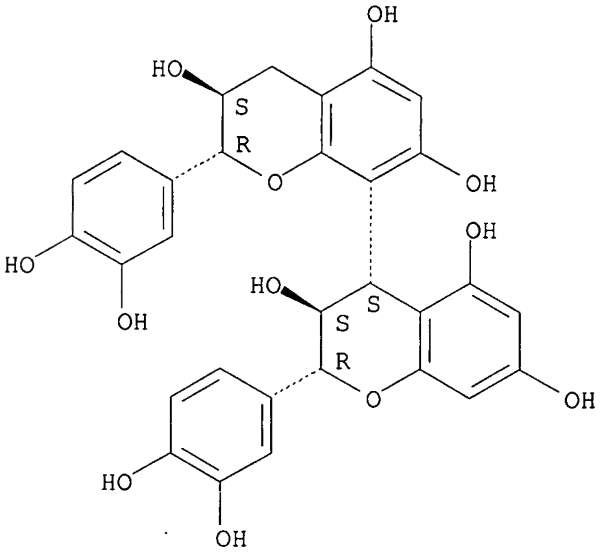
RN 20315-25-7 CAPLUS
CN [4,8'-Bi-2H-1-benzopyran]-3,3',5,5',7,7'-hexol, 2,2'-bis(3,4-dihydroxyphenyl)-3,3',4,4'-tetrahydro-, (2R,2'R,3R,3'S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



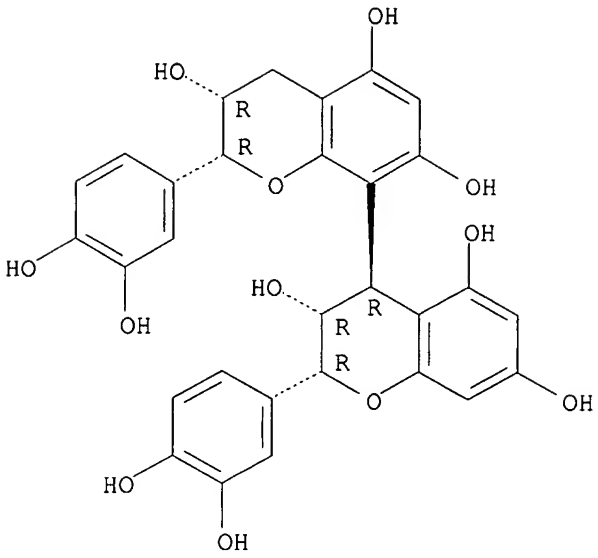
RN 23567-23-9 CAPLUS
CN [4,8'-Bi-2H-1-benzopyran]-3,3',5,5',7,7'-hexol, 2,2'-bis(3,4-dihydroxyphenyl)-3,3',4,4'-tetrahydro-, (2R,2'R,3S,3'S,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



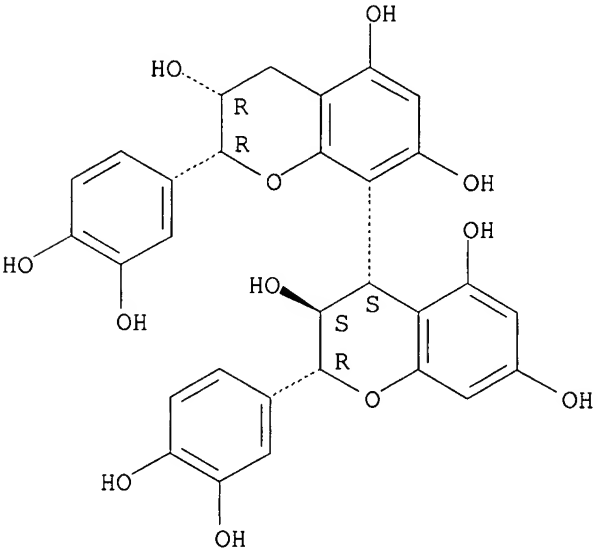
RN 29106-49-8 CAPLUS
CN [4,8'-Bi-2H-1-benzopyran]-3,3',5,5',7,7'-hexol, 2,2'-bis(3,4-dihydroxyphenyl)-3,3',4,4'-tetrahydro-, (2R,2'R,3R,3'R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 29106-51-2 CAPLUS
CN [4,8'-Bi-2H-1-benzopyran]-3,3',5,5',7,7'-hexol, 2,2'-bis(3,4-dihydroxyphenyl)-3,3',4,4'-tetrahydro-, (2R,2'R,3S,3'R,4S)- (9CI) (CA INDEX NAME)

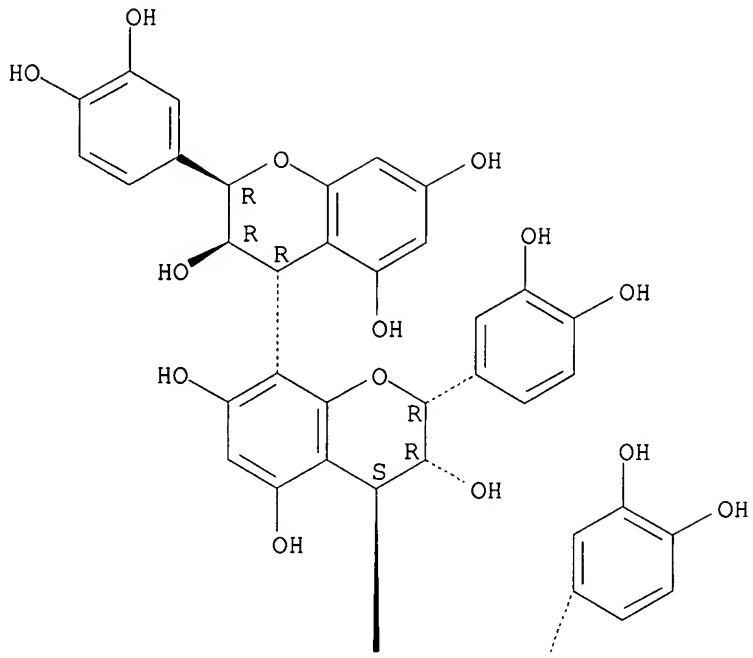
Absolute stereochemistry. Rotation (-).



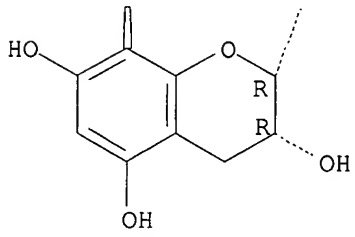
RN 37064-30-5 CAPLUS
CN [4,8':4',8''-Ter-2H-1-benzopyran]-3,3',3'',5,5',5'',7,7',7''-nonol, 2,2',2''-tris(3,4-dihydroxyphenyl)-3,3',3'',4,4',4''-hexahydro-, (2R,2'R,2''R,3R,3'R,3''R,4R,4'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

PAGE 1-A



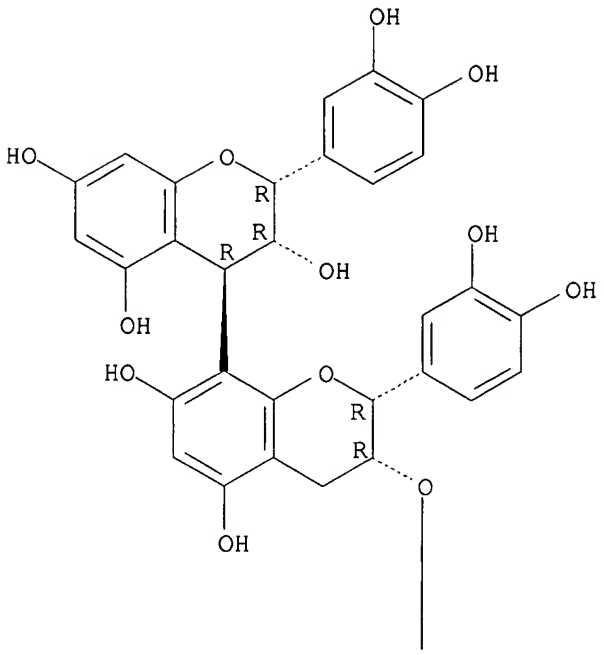
PAGE 2-A



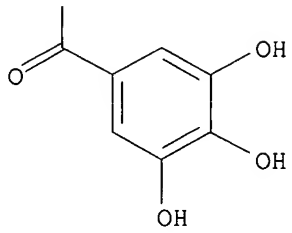
RN 73086-04-1 CAPLUS
CN Benzoic acid, 3,4,5-trihydroxy-, (2R,2'R,3R,3'R,4R)-2,2'-bis(3,4-dihydroxyphenyl)-3,3',4,4'-tetrahydro-3,5,5',7,7'-pentahydroxy[4,8'-bi-2H-1-benzopyran]-3'-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



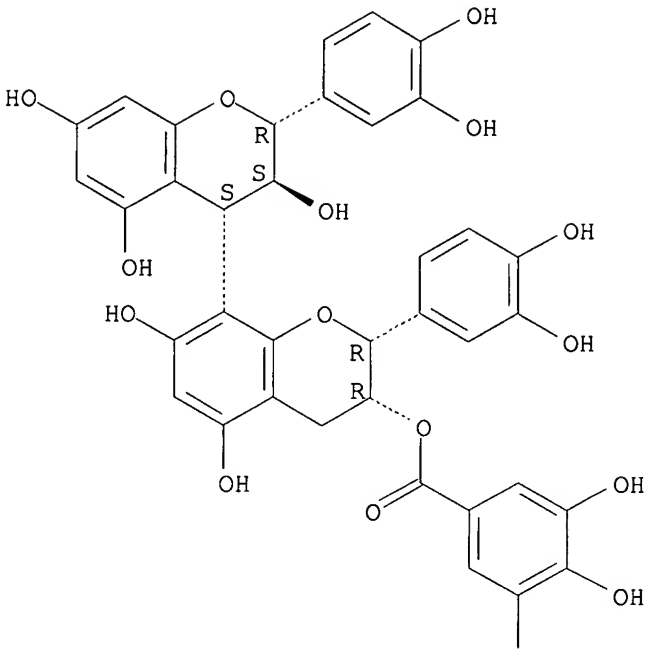
PAGE 2-A



RN 89064-33-5 CAPLUS
CN Benzoic acid, 3,4,5-trihydroxy-, (2R,2'R,3S,3'R,4S)-2,2'-bis(3,4-dihydroxyphenyl)-3,3',4,4'-tetrahydro-3,5,5',7,7'-pentahydroxy[4,8'-bi-2H-1-benzopyran]-3'-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

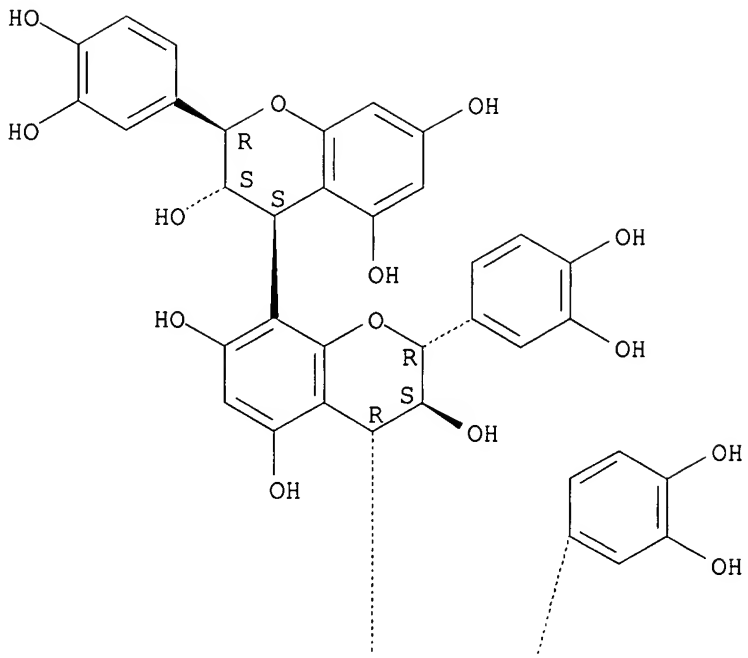


PAGE 2-A

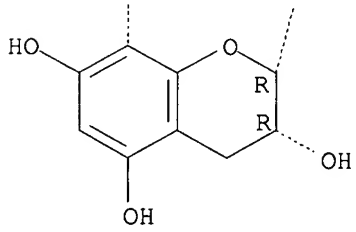
RN 97233-64-2 CAPLUS
CN [4,8':4',8''-Ter-2H-1-benzopyran]-3,3',3'',5,5',5'',7,7',7''-nonol, 2,2',2''-tris(3,4-dihydroxyphenyl)-3,3',3'',4,4',4''-hexahydro-, (2R,2'R,2''R,3S,3'S,3''R,4S,4'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



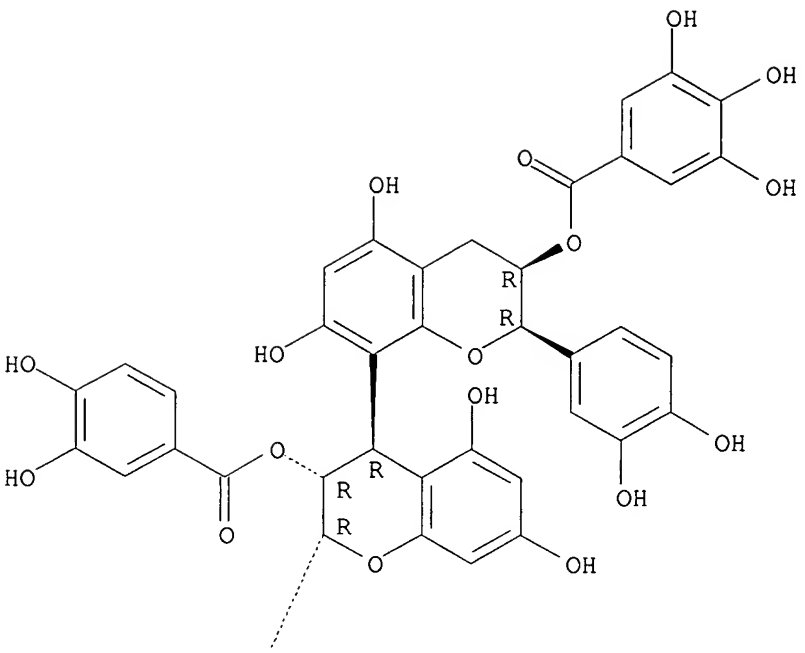
PAGE 2-A



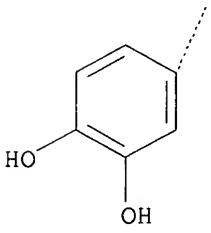
RN 201412-28-4 CAPLUS
CN Benzoic acid, 3,4,5-trihydroxy-, 3-[(3,4-dihydroxybenzoyl)oxy]-2,2'-bis(3,4-dihydroxyphenyl)-3,3',4,4'-tetrahydro-5,5',7,7'-tetrahydroxy[4,8'-bi-2H-1-benzopyran]-3'-yl ester, [2R-[2α,3α,4β(2'R*,3'R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



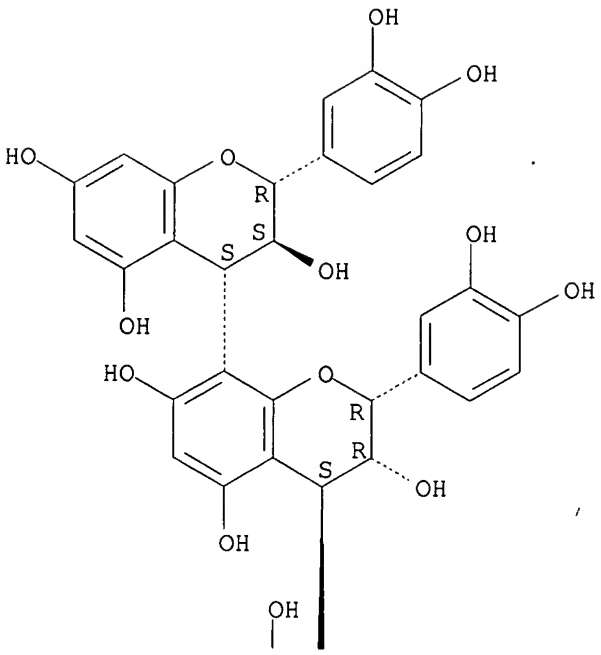
PAGE 2-A



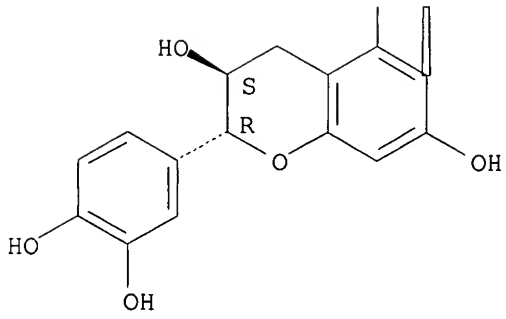
RN 202473-91-4 CAPLUS
CN [4,8':4',6''-Ter-2H-1-benzopyran]-3,3',3'',5,5',5'',7,7',7''-nonol, 2,2',2''-tris(3,4-dihydroxyphenyl)-3,3',3'',4,4',4''-hexahydro-, (2R,2'R,2''R,3S,3'R,3''S,4S,4'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A



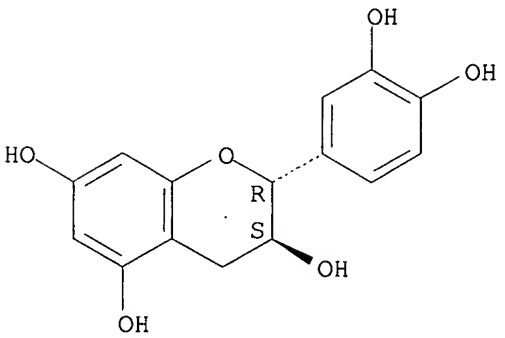
AB The kinetics of decomposition of the following flavan-3-ol derivs. isolated from grape seeds under oxidative conditions by airing and using metal ion catalysis (iron and copper) are determined: (+)-**catechin** and (-)-**epicatechin**; seven natural procyanidin **dimers**, B1 [(-)-**epicatechin**-(4→8)-(+)- **catechin**], B2 [(-)-**epicatechin**-(4→8)-(-)- **epicatechin**], B3 [(+)-**catechin**-(4→8)-(+)- **catechin**], B4 [(+)-**catechin**-(4→8)-(-)- **epicatechin**], B6 [(+)-**catechin**-(4→6)-(+)- **catechin**], B7 [(-)-**epicatechin**-(4→6)-(-)- **epicatechin**], and B8 [(-)-**epicatechin**-(4→8)-(-)- **epicatechin**]; trimers, C1 [(-)-**epicatechin**-(4→8)-(-)- **epicatechin** -(4→8)-(-)- **epicatechin**], (+)-**catechin** -(4→8)-(+)- **catechin**-(4→8)-(-)- **epicatechin** , and (+)-**catechin**-(4→8)-(-)- **epicatechin**

-(4→6)-(-)- **catechin**, monogallate esters of B2 and B4 and digallate of B2, which were isolated from grape seeds. Kinetic decomposition comparisons were monitored by HPLC. The following order was found for oxidative decomposition for procyanidin **dimers**: B3 ≈ B4 > B5 ≈ B6 > B1 ≈ B2 > B8. In the conditions of this study, the gallate ester of (-)-**epicatechin** is more unstable than (-)-**epicatechin**; inversely, kinetic decompns. of dimeric procyanidins B2 and B4 are much more important than those of their gallate esters. Mol. mechanics (MM2*) and 1H NMR studies of dimeric 3-O-gallate structures show a π-π stacking arrangement between the aromatic gallate and catechol rings, absent in analogous dimeric procyanidins, which reduces the total surface accessible to **oxidizing** agents.

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

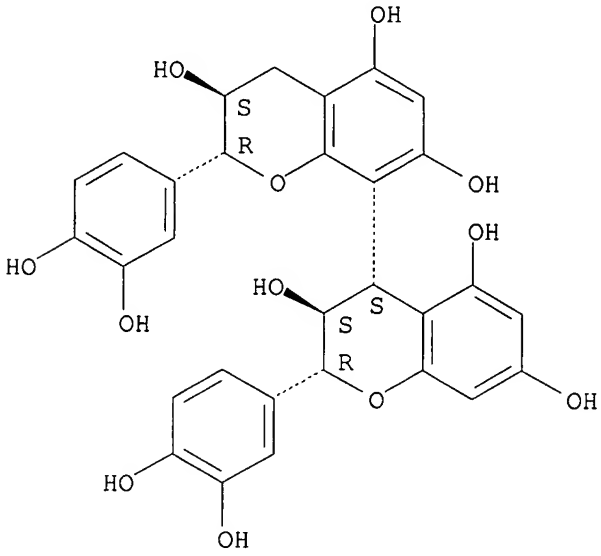
L10 ANSWER 20 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:465752 CAPLUS
DOCUMENT NUMBER: 125:189104
TITLE: Inhibition of β-glucosidase (Amygdalae dulces) by (+)-**catechin oxidation** products and procyanidin **dimers**
AUTHOR(S): Guyot, Sylvain; Pellerin, Patrice; Brillouet, Jean-Marc; Cheynier, Veronique
CORPORATE SOURCE: Laboratoire Polymeres Techniques Physico-Chimiques, IPV, Institut National Recherche Agronomique, Montpellier, 34060, Fr.
SOURCE: Bioscience, Biotechnology, and Biochemistry (1996), 60(7), 1131-1135
CODEN: BBBIEJ; ISSN: 0916-8451
PUBLISHER: Japan Society for Bioscience, Biotechnology, and Agrochemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **154-23-4**, (+)-**Catechin 23567-23-9**, Procyanidin B3 **29106-49-8**, Procyanidin B2 **36523-87-2** **73086-04-1 179185-59-2 179185-60-5**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(inhibition of β-glucosidase from almond by (+)- **catechin oxidation** products and procyanidin **dimers**)
RN 154-23-4 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



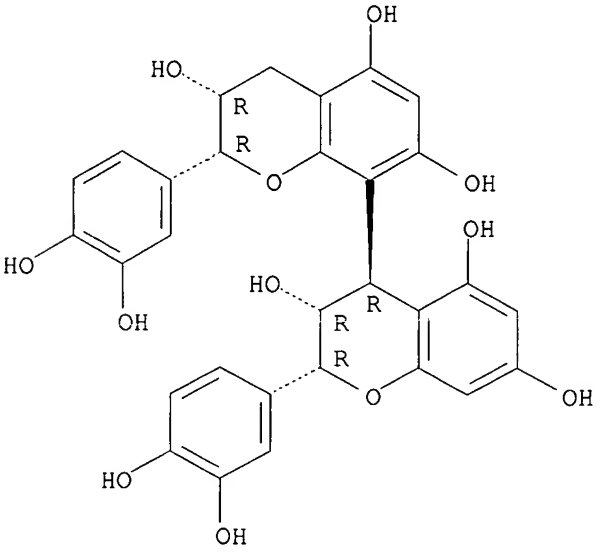
RN 23567-23-9 CAPLUS
CN [4,8'-Bi-2H-1-benzopyran]-3,3',5,5',7,7'-hexol, 2,2'-bis(3,4-dihydroxyphenyl)-3,3',4,4'-tetrahydro-, (2R,2'R,3S,3'S,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 29106-49-8 CAPLUS
CN [4,8'-Bi-2H-1-benzopyran]-3,3',5,5',7,7'-hexol, 2,2'-bis(3,4-dihydroxyphenyl)-3,3',4,4'-tetrahydro-, (2R,2'R,3R,3'R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

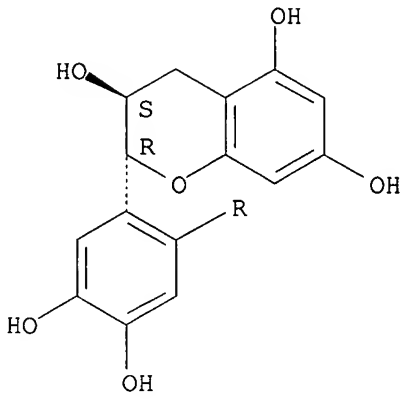


RN 36523-87-2 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 8-[2-[(2R,3S)-3,4-dihydro-3,5,7-trihydroxy-2H-

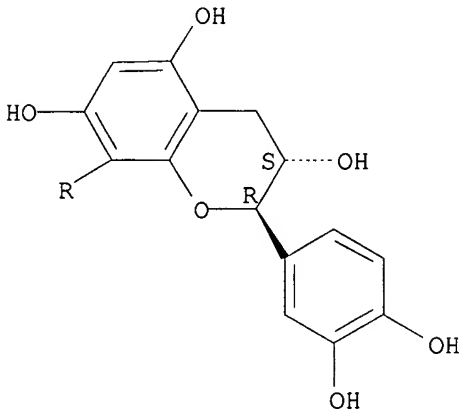
1-benzopyran-2-yl]-4,5-dihydroxyphenyl]-2-(3,4-dihydroxyphenyl)-3,4-dihydro-, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



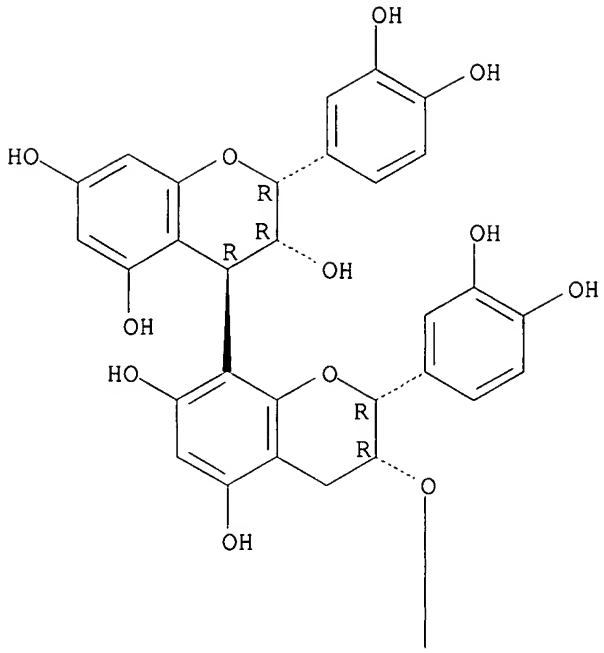
PAGE 2-A



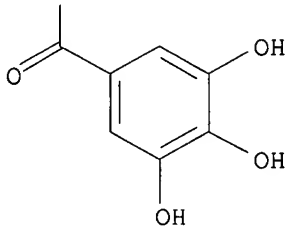
RN 73086-04-1 CAPLUS
CN Benzoic acid, 3,4,5-trihydroxy-, (2R,2'R,3R,3'R,4R)-2,2'-bis(3,4-dihydroxyphenyl)-3,3',4,4'-tetrahydro-3,5,5',7,7'-pentahydroxy[4,8'-bi-2H-1-benzopyran]-3'-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A

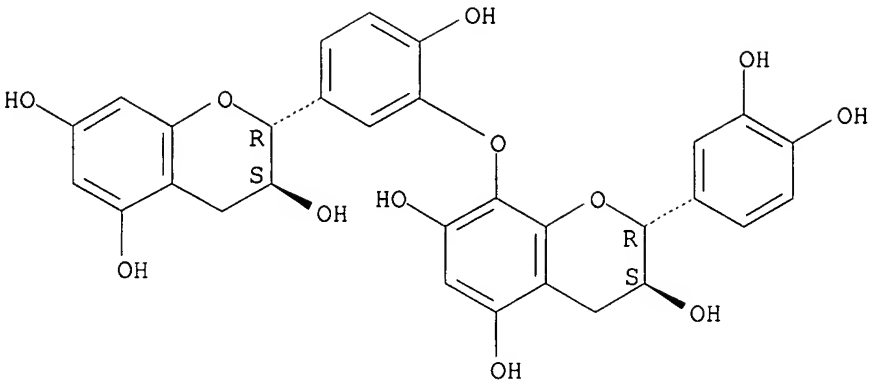


PAGE 2-A



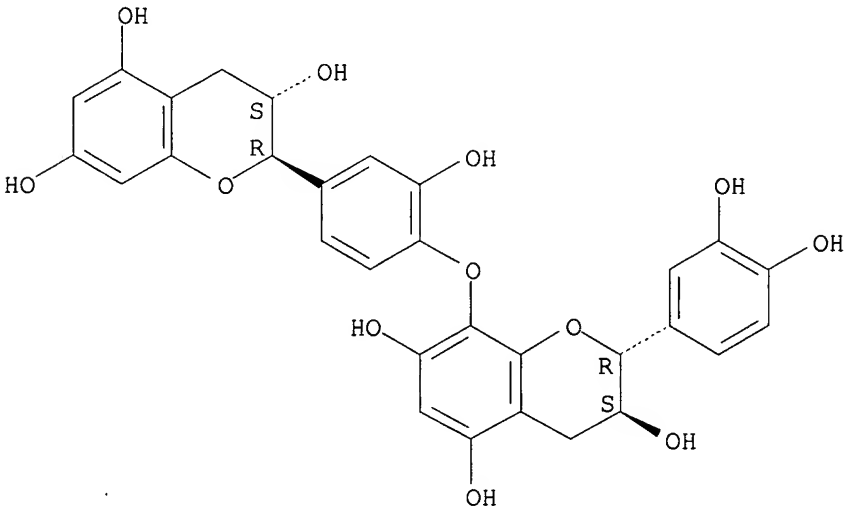
RN 179185-59-2 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 8-[5-(3,4-dihydro-3,5,7-trihydroxy-2H-1-benzopyran-2-yl)-2-hydroxyphenoxy]-2-(3,4-dihydroxyphenyl)-3,4-dihydro-, [2R-[2α,3β,8(2R*,3S*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 179185-60-5 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 8-[4-(3,4-dihydro-3,5,7-trihydroxy-2H-1-benzopyran-2-yl)-2-hydroxyphenoxy]-2-(3,4-dihydroxyphenyl)-3,4-dihydro-, [2R-[2α,3β,8(2R*,3S*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



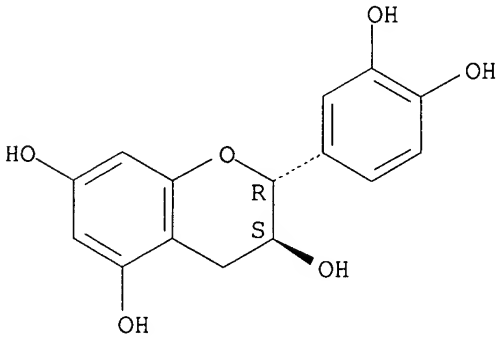
AB The sensitivity and specificity of the inhibition of β-glucosidase from almond (Amygdalae dulces) by (+)-**catechin**, an **oxidized** (+)-**catechin** solution, 3 dimeric procyanidins, and 5 (+)-**catechin dimers** obtained by enzymic **oxidation** were evaluated by using a chromatog. **method.** All of the polyphenols tested presented a significant inhibitory effect. Noncompetitive inhibition was observed for the **oxidized** (+)-**catechin** solution Some **oxidation** products were at least as powerful inhibitors as procyanidins which are known for their tanning effect. Yellow **oxidation** products were among the strongest inhibitors. No marked role of the number of OH and o-diphenol groups nor of the nature or position of the interflavanic linkage in the inhibitory effect was apparent.

L10 ANSWER 21 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:420728 CAPLUS

DOCUMENT NUMBER: 125:113062
TITLE: Structural determination of colorless and yellow **dimers** resulting from (+)-**catechin** coupling catalyzed by grape polyphenoloxidase
AUTHOR(S): Guyot, Sylvain; Vercauteren, Joseph; Cheynier, Veronique
CORPORATE SOURCE: Lab. Polym. Tech. Phys.-Chim., INRA, Montpellier, 34060, Fr.
SOURCE: Phytochemistry (1996), 42(5), 1279-1288
CODEN: PYTCAS; ISSN: 0031-9422
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **154-23-4**, (+)-**Catechin**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(structure of **dimers** resulting from (+)-**catechin** **oxidation** by grape polyphenoloxidase)
RN 154-23-4 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-, (2R,3S)- (9CI) (CA INDEX NAME)

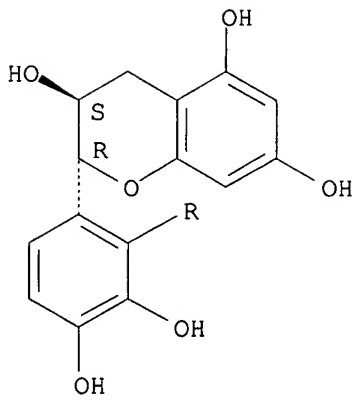
Absolute stereochemistry. Rotation (+).



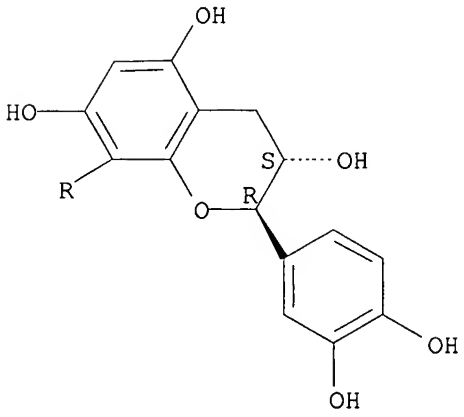
IT **64817-28-3 179185-59-2 179185-60-5 179185-61-6**
RL: BSU (Biological study, unclassified); MFM (Metabolic formation); PRP (Properties); BIOL (Biological study); FORM (Formation, nonpreparative)
(structure of **dimers** resulting from (+)-**catechin** **oxidation** by grape polyphenoloxidase)
RN 64817-28-3 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 8-[6-[(2R,3S)-3,4-dihydro-3,5,7-trihydroxy-2H-1-benzopyran-2-yl]-2,3-dihydroxyphenyl]-2-(3,4-dihydroxyphenyl)-3,4-dihydro-, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

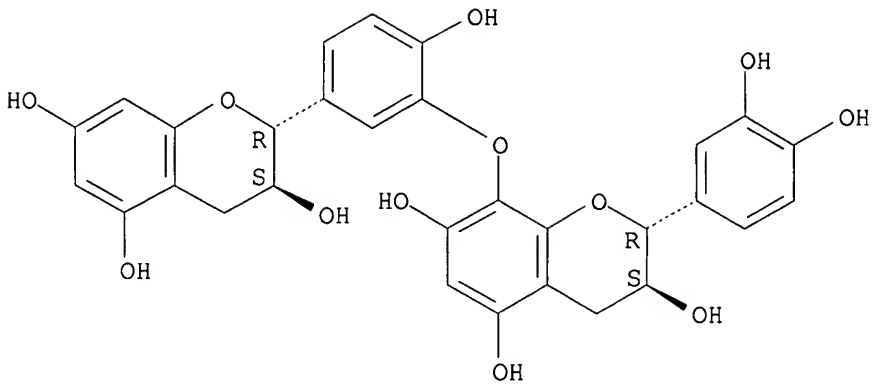


PAGE 2-A



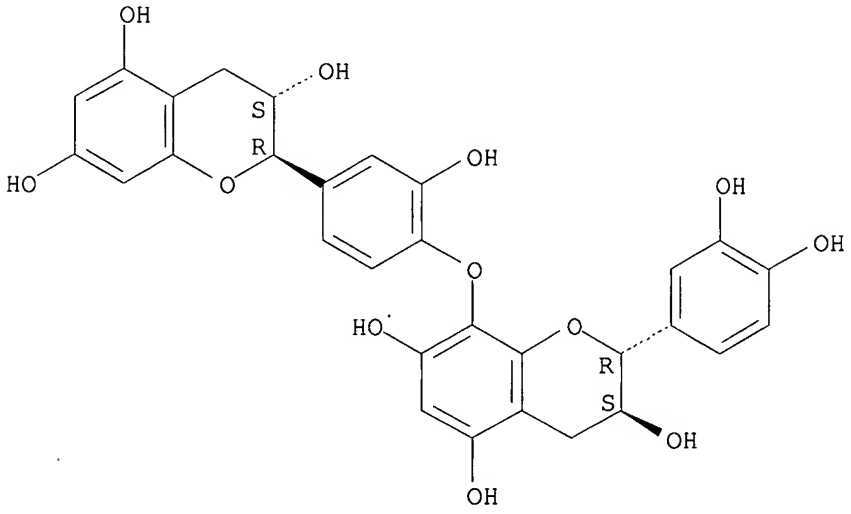
RN 179185-59-2 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 8-[5-(3,4-dihydro-3,5,7-trihydroxy-2H-1-benzopyran-2-yl)-2-hydroxyphenoxy]-2-(3,4-dihydroxyphenyl)-3,4-dihydro-, [2R-[2α,3β,8(2R*,3S*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



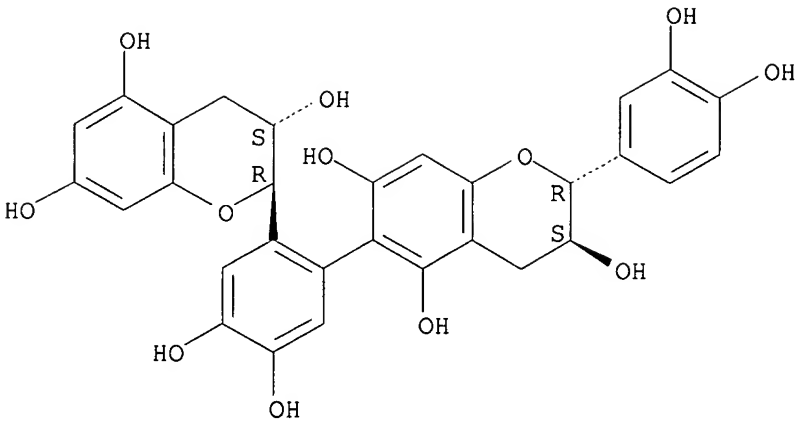
RN 179185-60-5 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 8-[4-(3,4-dihydro-3,5,7-trihydroxy-2H-1-benzopyran-2-yl)-2-hydroxyphenoxy]-2-(3,4-dihydroxyphenyl)-3,4-dihydro-, [2R-[2α,3β,8(2R*,3S*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



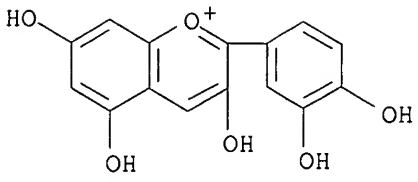
RN 179185-61-6 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 6-[2-[(2R,3S)-3,4-dihydro-3,5,7-trihydroxy-2H-1-benzopyran-2-yl]-4,5-dihydroxyphenyl]-2-(3,4-dihydroxyphenyl)-3,4-dihydro-, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



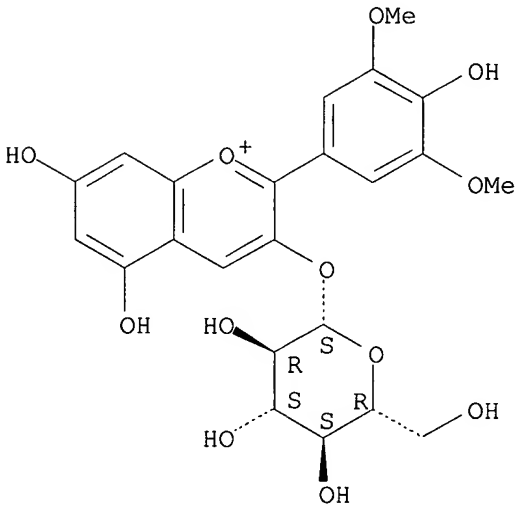
AB (+)-**Catechin oxidation** was carried out in aqueous systems using grape polyphenoloxidase as catalyst. Eight fractions corresponding to the major products formed at pH 3 and 6 were purified using HPLC at the **preparative** and semi-**preparative** scale. Structural characterization using UV-visible detection and mass spectrometry indicated that they corresponded to (+)-**catechin dimers** including two yellow pigments. Mono- and bi-dimensional 1H and 13C NMR analyses provided structural hypotheses for five **oxidation** products whereas the other three fractions were mixts. of several isomers. Colorless products, with C-C or C-O interflavan linkages, were dehydrodicatechins of the B-type. One of the two pigments corresponds to dehydrodicatechin A, already identified in other **oxidation** models, and the other pigment is a new structure of the quinone-methide type.

L10 ANSWER 22 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:140282 CAPLUS
DOCUMENT NUMBER: 124:200664
TITLE: Principal phenolic phytochemicals in French Syrah and Grenache Rhone wines and their antioxidant activity in inhibiting **oxidation** of human low density lipoproteins
AUTHOR(S): Teissedre, P-. L.; Waterhouse, A. L.; Frankel, E. N.
CORPORATE SOURCE: Faculte de Pharmacie, Universite de Montpellier I, Montpellier, 34060, Fr.
SOURCE: Journal International des Sciences de la Vigne et du Vin (1995), 29(4), 205-12
CODEN: JISVE8; ISSN: 1151-0285
PUBLISHER: Vigne et Vin Publications Internationales
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **528-58-5**, Cyanidin **7228-78-6**, Malvidin-3-glucoside
20315-25-7, Procyanidin B1 **23567-23-9**, Procyanidin B3
29106-49-8, Procyanidin B2
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(phenolic constituents in French Syrah and Grenache Rhone wines and their antioxidant activities in inhibiting **oxidation** of human low d. lipoproteins)
RN 528-58-5 CAPLUS
CN 1-Benzopyrylium, 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-, chloride (9CI) (CA INDEX NAME)



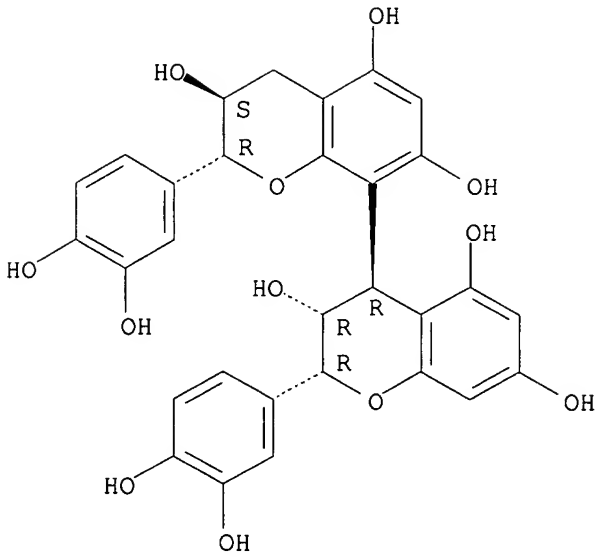
RN 7228-78-6 CAPLUS
CN 1-Benzopyrylium, 3-(β-D-glucopyranosyloxy)-5,7-dihydroxy-2-(4-hydroxy-3,5-dimethoxyphenyl)-, chloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



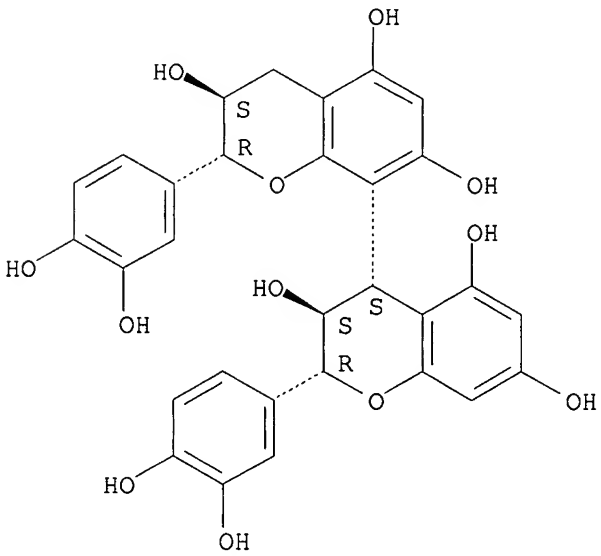
RN 20315-25-7 CAPLUS
CN [4,8'-Bi-2H-1-benzopyran]-3,3',5,5',7,7'-hexol, 2,2'-bis(3,4-dihydroxyphenyl)-3,3',4,4'-tetrahydro-, (2R,2'R,3R,3'S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



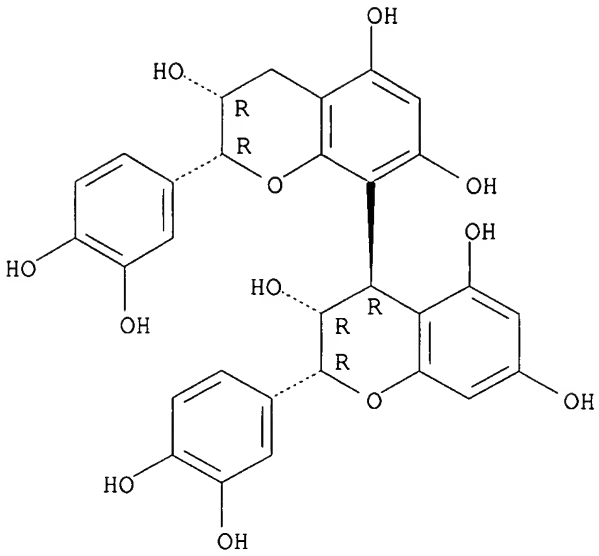
RN 23567-23-9 CAPLUS
CN [4,8'-Bi-2H-1-benzopyran]-3,3',5,5',7,7'-hexol, 2,2'-bis(3,4-dihydroxyphenyl)-3,3',4,4'-tetrahydro-, (2R,2'R,3S,3'S,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 29106-49-8 CAPLUS
CN [4,8'-Bi-2H-1-benzopyran]-3,3',5,5',7,7'-hexol, 2,2'-bis(3,4-dihydroxyphenyl)-3,3',4,4'-tetrahydro-, (2R,2'R,3R,3'R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



AB Wine contains natural plant phenolic antioxidants that may protect circulating lipoproteins from oxidative damage. By inhibition of the copper-catalyzed **oxidation** of LDL, we determined the activity of thirteen Rhone Coast wines exclusively from Syrah and Grenache varieties. About 50% of the wines were **made** with a long maceration **process**. Major monomeric phenolic compds. and procyanidin **dimers** were analyzed in each sample by HPLC and correlated with relative LDL antioxidant activity. Correlations obtained can be grouped in 3 classes: **catechin** (r = 0.75), procyanidins B1, B2, and B3 (r = 0.43-0.55), malvidin-3-glucoside and cyanidin (r = 0.43), gallic acid, myricetin, rutin (r = 0.2-0.4). On the same basis total phenol contents of wines gave a correlation with LDL antioxidant activity of r = 0.72. Comparison, at the same total phenol concentration, with different red California wines shows that antioxidant activity of French Syrah and Grenache range between that of Merlot (56-65%) and Cabernet Sauvignon (37-45%). In contrast Syrah wines **made** with a short extraction **process** gave lower inhibition of LDL **oxidation** of 16% which is less than white California wines averaging 36%. Activity of each wine phenolic compound can play a role in protecting LDL against **oxidation**

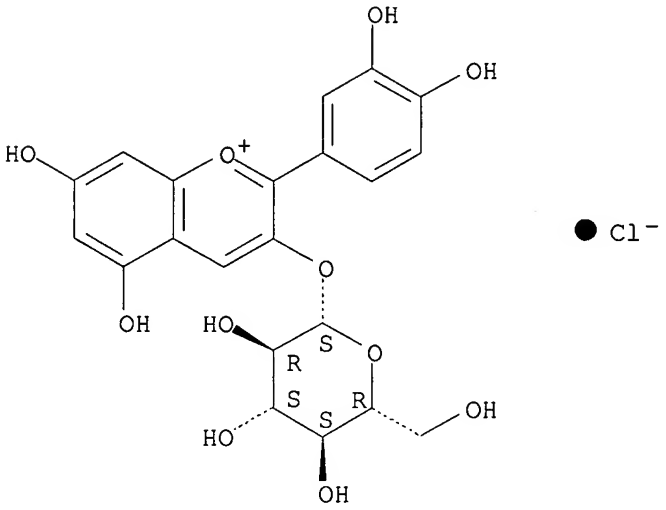
L10 ANSWER 23 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:792395 CAPLUS
DOCUMENT NUMBER: 123:197162
TITLE: Reactions of enzymically generated quinones in relation to browning in grape musts and wines
AUTHOR(S): Cheynier, Veronique; Fulcrand, Helene; Guyot, Sylvain; Oszmianski, Jan; Moutounet, Michel
CORPORATE SOURCE: Laboratoire des Polymeres et des Technique Physico-chimiques, Institut National de la Recherche Agronomique, Montpellier, 34060, Fr.
SOURCE: ACS Symposium Series (1995), 600(Enzymatic Browning and Its Prevention), 130-43
CODEN: ACSMC8; ISSN: 0097-6156
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **7084-24-4**, Cyanidin-3-glucoside

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(reactions of enzymically generated quinones in relation to browning in grape musts and wines)

RN 7084-24-4 CAPLUS

CN 1-Benzopyrylium, 2-(3,4-dihydroxyphenyl)-3-(β-D-glucopyranosyloxy)-5,7-dihydroxy-, chloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

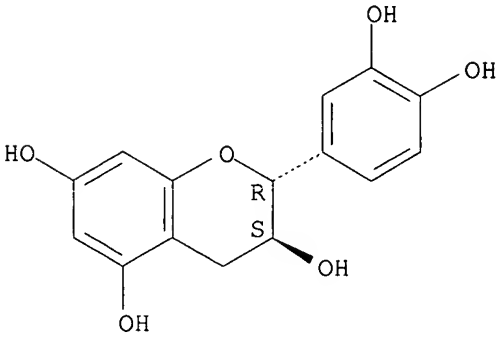


IT **154-23-4**, (+)-**Catechin 7228-78-6**, Malvidin-3-glucoside
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactions of enzymically generated quinones in relation to browning in grape musts and wines)

RN 154-23-4 CAPLUS

CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-, (2R,3S)- (9CI) (CA INDEX NAME)

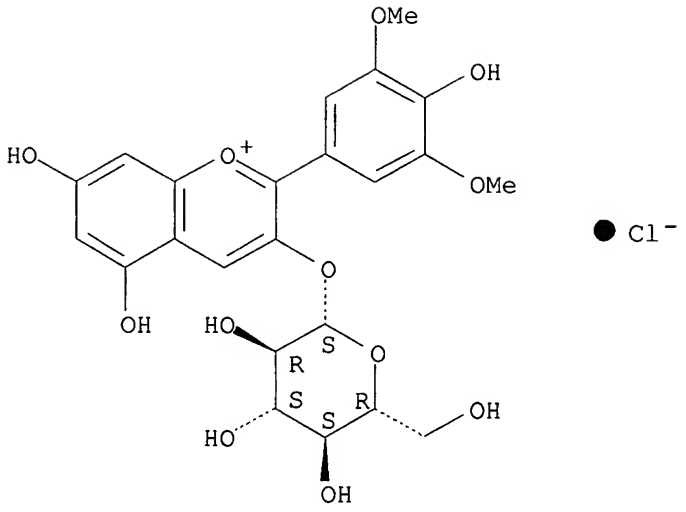
Absolute stereochemistry. Rotation (+).



RN 7228-78-6 CAPLUS

CN 1-Benzopyrylium, 3-(β-D-glucopyranosyloxy)-5,7-dihydroxy-2-(4-hydroxy-3,5-dimethoxyphenyl)-, chloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

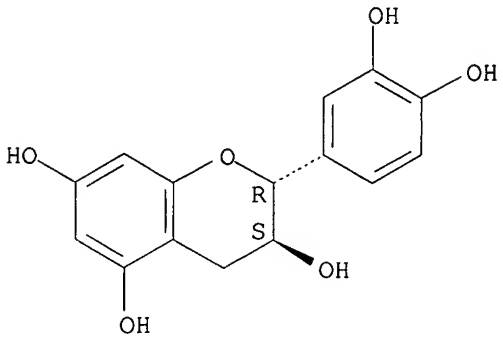


AB The role of enzymically generated caffeoyltartaric acid quinones in browning development was investigated in grape musts and model solns. Caffeoyltartaric acid quinones are only slightly colored and undergo condensation rather slowly, yielding mostly colorless products. On the other hand, they are powerful oxidants and, in particular, **oxidize** flavan-3-ols to unstable secondary quinones which proceed readily to brown polymers. The structures of **dimers** resulting from caffeic acid **oxidation** were elucidated, and the involvement of nucleophilic attack by water in the **process** of their formation demonstrated. Seven **dimers**, including both colorless and brown compds., were obtained by **oxidation** of **catechin** and characterized. The involvement of caffeoyltartaric acid quinone in anthocyanin oxidative degradation was also established. Trapping of primary quinones by glutathione competes with reactions leading to must discoloration but maintains high levels of **oxidizable** compds., especially flavan-3-ols, which serve as browning precursors in wine.

L10 ANSWER 24 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1984:470941 CAPLUS
DOCUMENT NUMBER: 101:70941
TITLE: Turbidity formed in beer at low temperatures. Affinity of proanthocyanidins and their **oxidation** products for haze-forming proteins of beer and the formation of chill haze
AUTHOR(S): Asano, Katsuhiko; Ohtsu, Keiji; Shinagawa, Kyoko; Hashimoto, Naoki
CORPORATE SOURCE: Brew. Sci. Lab., Kirin Brew. Co., Ltd., Takasaki, 370-12, Japan
SOURCE: Agricultural and Biological Chemistry (1984), 48(5), 1139-46
CODEN: ABCHA6; ISSN: 0002-1369
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **154-23-4 490-46-0 23567-23-9 37064-31-6**
RL: PRP (Properties)
(protein affinity of, of beer, chill haze in relation to)
RN 154-23-4 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-,

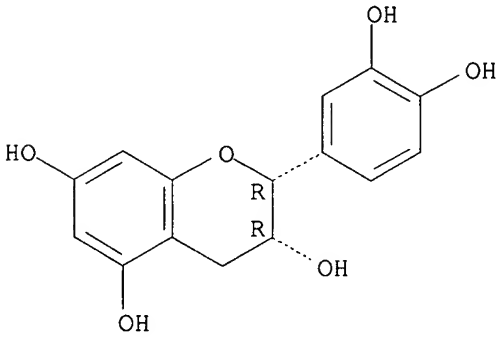
(2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



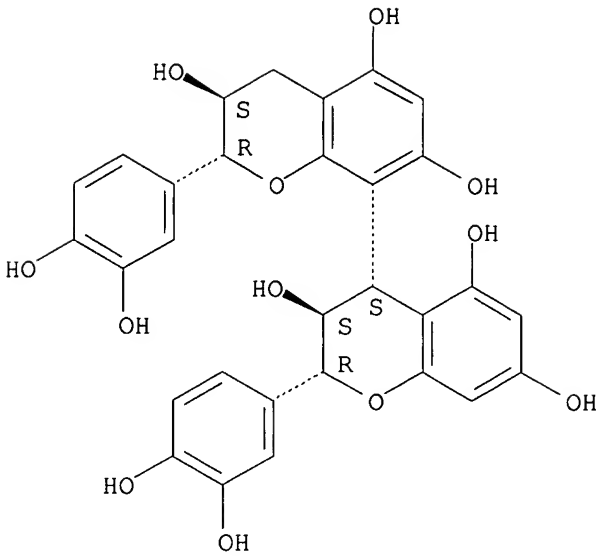
RN 490-46-0 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 23567-23-9 CAPLUS
CN [4,8'-Bi-2H-1-benzopyran]-3,3',5,5',7,7'-hexol, 2,2'-bis(3,4-dihydroxyphenyl)-3,3',4,4'-tetrahydro-, (2R,2'R,3S,3'S,4S)- (9CI) (CA INDEX NAME)

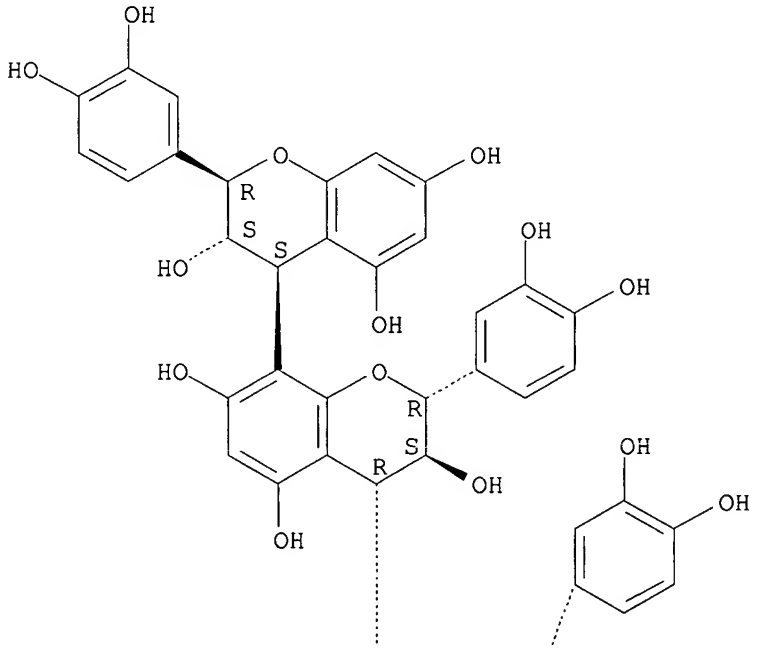
Absolute stereochemistry. Rotation (-).



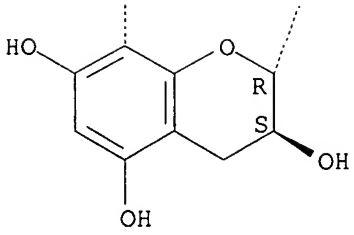
RN 37064-31-6 CAPLUS
CN [4,8':4',8''-Ter-2H-1-benzopyran]-3,3',3'',5,5',5'',7,7',7''-nonol, 2,2',2''-tris(3,4-dihydroxyphenyl)-3,3',3'',4,4',4''-hexahydro-, (2R,2'R,2''R,3S,3'S,3''S,4R,4'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



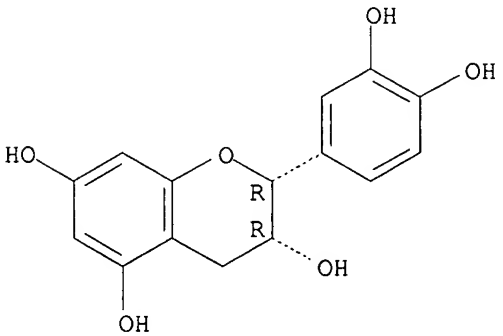
PAGE 2-A



AB Among the polyphenols found in beer, proanthocyanidins have a specific affinity for the haze-forming proteins in beer and retained their capacity to form a chill haze. Proanthocyanidin pentamer and tetramer had the highest affinities for the haze-forming proteins, followed by trimer, **dimer**, and **catechins**. During the brewing **process**, proanthocyanidin trimer and polymeric proanthocyanidins easily formed insol. complexes with proteins in the wort as a result of their high affinity for proteins; consequently, these were not found in finished beer, whereas such proanthocyanidin **dimers** as procyanidin B3 [**23567-23-9**], and **catechin** [**154-23-4**] survived in finished beer. Procyanidin B3 and **catechin**, when stored in beer or a buffer solution, seemed to undergo oxidative polymerization and increased their affinity for the haze-forming proteins to form a extensive chill haze.

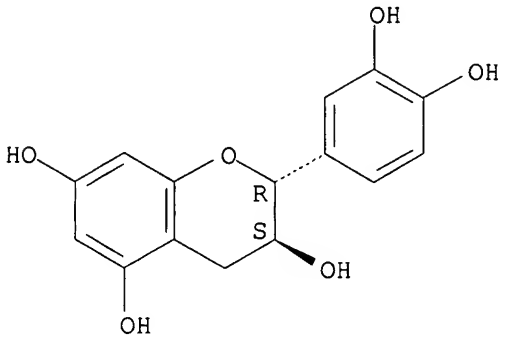
L10 ANSWER 25 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1981:619585 CAPLUS
DOCUMENT NUMBER: 95:219585
TITLE: Stability of (+)-cyanidanol-3 in aqueous solution
AUTHOR(S): Akimoto, Koichi; Sugimoto, Isao
CORPORATE SOURCE: Pharm. Res. Cent., Kanebo Ltd., Osaka, 534, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1981), 29(7), 2005-11
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **490-46-0P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, from cyanidanol, kinetics of)
RN 490-46-0 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



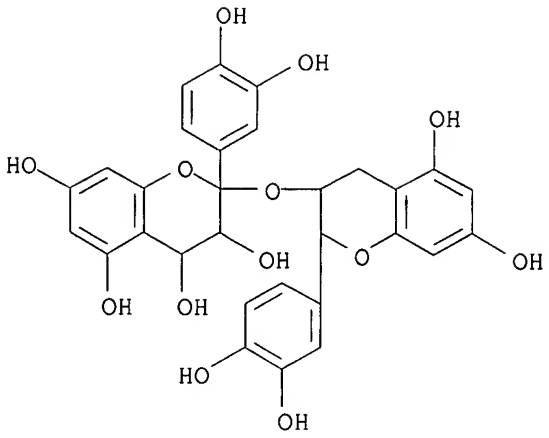
IT **154-23-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactions of, in aqueous solution)
RN 154-23-4 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



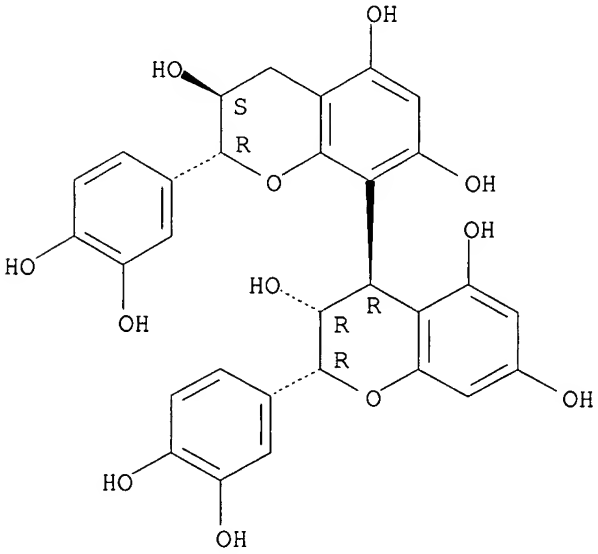
AB Two degradation products were obtained from the title compound (I) at pH 1.4: **epicatechin** (II) and the **dimer**. In the basic pH region, the main product was II. The effect of O was remarkable, especially in basic solution In strongly acidic solution, the degradation of I occurred by simultaneous apparent 1st-order (epimerization) and 2nd-order (dimerization) reactions. The rate consts. were calculated by a new **method**. In the neutral and basic pH regions, the reverse reaction between I and II took place and the rate consts. were obtained.

L10 ANSWER 26 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1980:56776 CAPLUS
DOCUMENT NUMBER: 92:56776
TITLE: The procyanidins of white grapes and wines
AUTHOR(S): Lea, Andrew G. H.; Bridle, Peter; Timberlake, Colin F.; Singleton, Vernon L.
CORPORATE SOURCE: Long Ashton Res. Stn., Univ. Bristol, Long Ashton/Bristol, BS18 9AF, UK
SOURCE: American Journal of Enology and Viticulture (1979), 30(4), 289-300
CODEN: AJEVAC; ISSN: 0002-9254
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **4852-22-6D**, derivs. **20315-25-7 23567-23-9 29106-49-8 29106-51-2**
RL: BIOL (Biological study)
(of grapes and wines)
RN 4852-22-6 CAPLUS
CN 2H-1-Benzopyran-3,4,5,7-tetrol, 2-(3,4-dihydroxyphenyl)-2-[[2-(3,4-dihydroxyphenyl)-3,4-dihydro-5,7-dihydroxy-2H-1-benzopyran-3-yl]oxy]-3,4-dihydro- (9CI) (CA INDEX NAME)



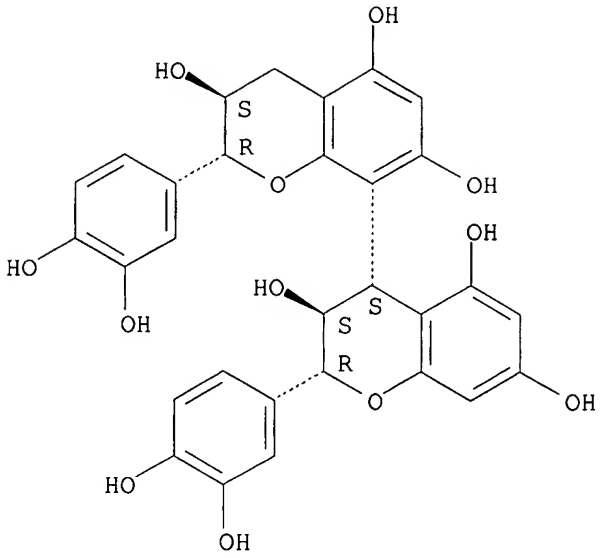
RN 20315-25-7 CAPLUS
CN [4,8'-Bi-2H-1-benzopyran]-3,3',5,5',7,7'-hexol, 2,2'-bis(3,4-dihydroxyphenyl)-3,3',4,4'-tetrahydro-, (2R,2'R,3R,3'S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



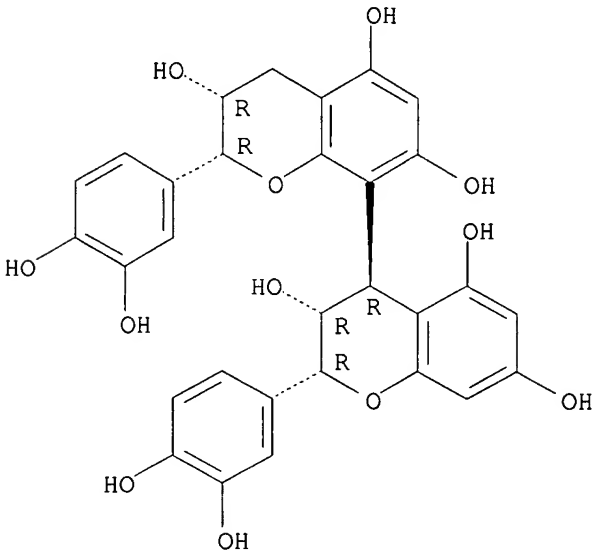
RN 23567-23-9 CAPLUS
CN [4,8'-Bi-2H-1-benzopyran]-3,3',5,5',7,7'-hexol, 2,2'-bis(3,4-dihydroxyphenyl)-3,3',4,4'-tetrahydro-, (2R,2'R,3S,3'S,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



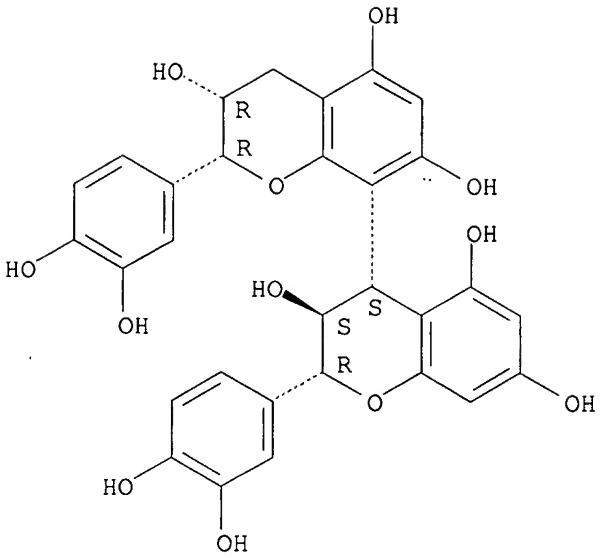
RN 29106-49-8 CAPLUS
CN [4,8'-Bi-2H-1-benzopyran]-3,3',5,5',7,7'-hexol, 2,2'-bis(3,4-dihydroxyphenyl)-3,3',4,4'-tetrahydro-, (2R,2'R,3R,3'R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 29106-51-2 CAPLUS
CN [4,8'-Bi-2H-1-benzopyran]-3,3',5,5',7,7'-hexol, 2,2'-bis(3,4-dihydroxyphenyl)-3,3',4,4'-tetrahydro-, (2R,2'R,3S,3'R,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

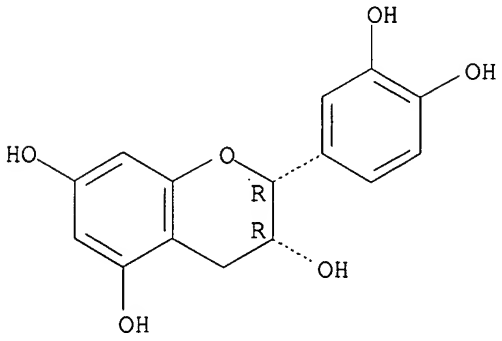


AB Procyanidin exts. were **prepared** from a Seyval white wine, from a Mueller-Thurgau wine fermented partly on its skins, and from grape seeds. The exts. were studied chromatog. and revealed a range of discrete procyanidin oligomers up to the pentameric and significant quantities of more polymeric and **oxidized** material. Semiquant. estns. showed that the level of total procyanidins was as low as 5-10 mg/L in the Seyval wine rising to 300 mg/L in the Mueller-Thurgau, but that the qual. distribution patterns of the **catechins** and procyanidins showed no marked differences between the two. The Mueller-Thurgau extract was examined counter-current distribution between EtOAc and H2O, thus achieving a separation of different groups of oligomeric procyanidins, and this was followed by further chromatog. treatment on Sephadex LH-20. The 4 main procyanidin **dimers** of white wines were isolated in the free state and were characterized by chromatog. and their degradative behavior in the presence of acidic toluene-thiol as procyanidins B1-B4. A further procyanidin fraction was isolated and shown to consist of a mixture of 2 stereoisomeric trimers, 1 composed of 3 **epicatechin** units and the other of 2 **epicatechins** and a terminal **catechin**. The English-grown Mueller-Thurgau wine contained negligible amts. of gallocatechins and of galloyl esters of **catechins**, either alone or in combination as procyanidins; this is in contrast to some previous reports.

L10 ANSWER 27 OF 27 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1965:433098 CAPLUS
DOCUMENT NUMBER: 63:33098
ORIGINAL REFERENCE NO.: 63:5944f-h,5945a
TITLE: Suitability of sulfurous acid for hydrolysis of condensed tannins
AUTHOR(S): Quesnel, V. C.
CORPORATE SOURCE: Univ. West Indies, St. Augustine, Trinidad
SOURCE: Tetrahedron Letters (1964), (48), 3699-702
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **490-46-0**, Epicatechol
(from Cacao leucocyanidin polymer)

RN 490-46-0 CAPLUS
CN 2H-1-Benzopyran-3,5,7-triol, 2-(3,4-dihydroxyphenyl)-3,4-dihydro-, (2R,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



AB Although condensed tannins are hydrolyzed by dilute acids, concomitant acid-catalyzed polymerization occurs. Alkaline hydrolysis is complicated by oxidative condensation. The suitability of H2SO3, as suggested by Forsyth and Roberts (CA 54, 14238b) in a study of the hydrolysis of leucocyanidin **dimer**, for investigations on the structure of condensed tannins was examined Acid-catalyzed polymers were **prepared** according to the **method** of Goldstein and Swain (CA 60, 2046d) and the precipitated polymers collected by filtration. **Oxidation** polymers were **prepared** from 100-mg. samples in 50 ml. H2O by overnight **oxidation** at 20° with 75 mg. NaIO4; the solns. were saturated with salt and the polymers collected on sintered glass. Cacao polyphenyl storage cells (Brown, Nature 173(4402), 492(1954)) and mangrove bark, extracted with MeOH and the exts. diluted with 2 vols. Et2O, gave cacao and mangrove tannins, resp. Polymerization by acid and by **oxidation** gave (-)-**epicatechin** polymers (I, II) and cacao leucocyanidins 1 and 2 polymers (III, IV). Extraction gave polymeric cacao leucocyanidin (V, VI) from cacao and mangrove tannin, resp. I and II were practically insol. in H2O; the others were H2O-soluble I was partially and III wholly soluble in EtOH. On 2-way chromatography in 2% aqueous AcOH and a BuOH phase of 4:1:5 BuOH-AcOH-H2O, none showed any discreet spot in both solvents. The polymers were refluxed in aqueous or alc. H2SO3 for 2.5 hrs. and again examined chromatograpically. No spot mobile in both solvents was produced from I, III, or IV, but the others gave mobile spots. II was split to give a spot with Rf 0.02 (2% aqueous HOAc), 0.5 (BuOH-HOAc-H2O, 4:1:5) and another with Rf 0.95 (aqueous HOAc), 0.5 (BuOH). V was completely split into (-)-**epicatechin**, substance A, and substance B. Longer treatment gave complete hydrolysis to substance A, (-)-**epicatechin**, and (+)-**catechin**. Hydrolysis of VI was extensive. The bulk of VI was closely similar to that of V and it is possible that other condensed tannins are similar to V. The use of H2SO3 in their structural investigations was suggested. Quebracho tannin is extensively altered by bisulfite treatment.

=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	180.54	347.69

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL

	ENTRY	SESSION
CA SUBSCRIBER PRICE	-20.25	-20.25

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